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FILE LAST UPDATED: 11 Aug 2005  (20050811/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

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L1               STR
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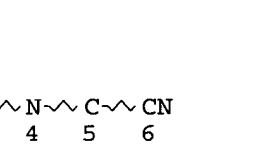


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DEFAULT ECLEVEL IS LIMITED

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RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
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L6               STR
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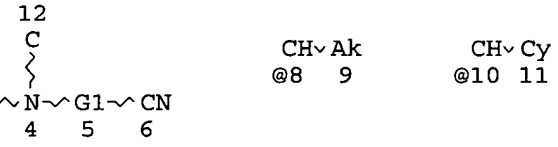


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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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L9       359971 SEA FILE=HCAPLUS ABB=ON  PLU=ON  DIABETE?/CV OR (HYPERGLYCEMIA/
                CV OR GLUCEMIA/CV OR "GLYCEMIA OR GLUCEMIA"/CV OR "HIGH BLOOD
                GLUCOSE"/CV OR "HIGH BLOOD SUGAR"/CV OR "ANTIDIABETIC AGENTS"/C
                V OR "DIABETES MELLITUS"/CV OR GLUCOSE/CV OR INSULIN/CV) OR
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                ?GLYCEM?
L10           5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND L9


=>
=>

=> d ibib abs hitstr l10 1-5

L10  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2005:371023  HCAPLUS
DOCUMENT NUMBER:          142:430272
TITLE:                    Preparation of 3,5-disubstituted indazoles with
                          nitrogen-bearing 5-membered heterocycles for mediating
                          or inhibiting cell proliferation
INVENTOR(S):              McAlpine, Indrawan James; Deal, Judith Gail; Johnson,
                          Mary Catherine; Kephart, Susan Elizabeth; Park, Julie
                          Yongsun; Romines, William Henry; Tikhe, Jayashree G.
PATENT ASSIGNEE(S):       Pfizer Inc, USA
SOURCE:                   U.S. Pat. Appl. Publ., 184 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     US 2005090529         A1    20050428    US 2004-910217           20040802
PRIORITY APPLN. INFO.:                       US 2003-491821P      P   20030731
OTHER SOURCE(S):          MARPAT 142:430272
GI
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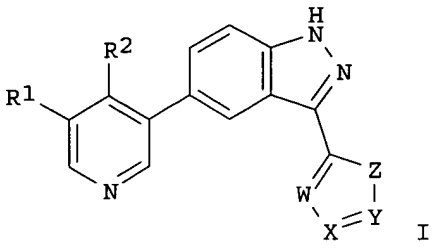


I

AB The title indazoles I with substituted nitrogen bearing 5-membered heterocycles in the 3-position [I; W = C, N; X and Y = N, CR3, CR4; Z = C, NH, O, S; R1, R2 = H, alkyl, (un)substituted NH2, etc.; R3, R4 = H, halo, CN, etc.] that modulate and/or inhibit cell proliferation, such as the activity of protein kinases, were prepared E.g., a multi-step synthesis of I [W = N; Z = NH; X, Y = CH; R1 = CH2NHEt; R2 = Me], starting from 5-bromo-4-methylpyridine-3-carboxaldehyde, was given. The compds. I and pharmaceutical compns. containing them are capable of mediating CDK dependent diseases to modulate and/or inhibit unwanted cell proliferation (the Ki values against CDK2 were given). The invention is also directed to the therapeutic or prophylactic use of pharmaceutical compns. containing such compds. I, and to methods of treating cancer as well as other disease states associated with unwanted angiogenesis and/or cellular proliferation, such as **diabetic** retinopathy, neovascular glaucoma, rheumatoid arthritis, and psoriasis, by administering effective amts. of such compds.

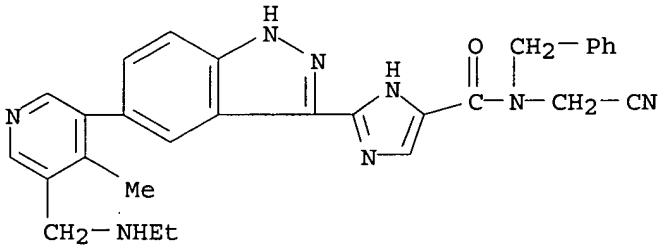
IT **850891-21-3P**

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 3,5-disubstituted indazoles with nitrogen-bearing 5-membered heterocycles for mediating or inhibiting cell proliferation)

RN 850891-21-3 HCAPLUS

CN 1H-Imidazole-4-carboxamide, N-(cyanomethyl)-2-[5-[5-[(ethylamino)methyl]-4-methyl-3-pyridinyl]-1H-indazol-3-yl]-N-(phenylmethyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:259865 HCAPLUS

DOCUMENT NUMBER: 142:336644

TITLE: Preparation of amino acid derivatives as dipeptidyl peptidase IV inhibitors

INVENTOR(S): Tsutsumi, Kazuhiro; Shinkai, Hisashi; Kitao, Yuki; Yamashita, Masaki; Kobayashi, Satoru; Matsui, Kenichi; Oda, Tomohiro; Taniguchi, Toshio; Asahina, Kota

PATENT ASSIGNEE(S): Japan Tobacco Inc., Japan
SOURCE: PCT Int. Appl., 356 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005025554	A2	20050324	WO 2004-JP13480	20040909

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:		
JP 2003-317407	A	20030909
JP 2003-395879	A	20031126
JP 2004-114685	A	20040408

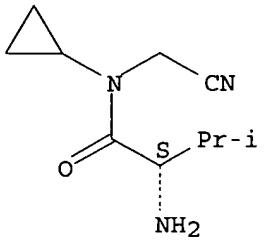
OTHER SOURCE(S): MARPAT 142:336644

AB The invention relates to amino acid amides R1NHCR4R5CONR2R3 [R1, R2 = H, (un)substituted alkyl or cycloalkyl; R3 = (un)substituted alkyl or cycloalkyl; R4, R5 = H, (un)substituted alkyl, cycloalkyl, aryl, aralkyl, heterocyclyl or heterocyclylalkyl], including stereoisomers or pharmaceutically-acceptable salts, which show dipeptidyl peptidase IV (DPP-IV) inhibitory activity and are effective for the treatment of type II **diabetes**, obesity, etc. Thus, (2S)-N-cyclobutyl-N-methyl-2-amino-2-cyclohexylacetamide hydrochloride, prepared by amidation reaction, showed IC50 < 10 μM for inhibition of DPP-IV.

IT **848493-98-1P 848493-99-2P 848494-00-8P**
848494-01-9P 848494-03-1P 848494-10-0P
848494-11-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of amino acid derivs. as dipeptidyl peptidase IV inhibitors)

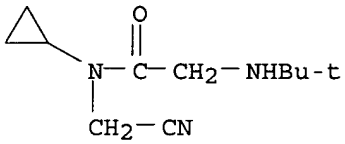
RN 848493-98-1 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-N-cyclopropyl-3-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



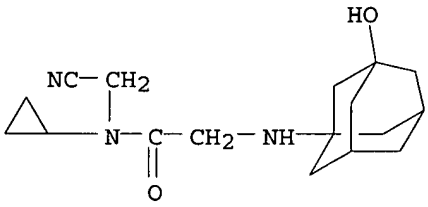
● HCl

RN 848493-99-2 HCAPLUS
CN Acetamide, N-(cyanomethyl)-N-cyclopropyl-2-[(1,1-dimethylethyl)amino]-, monohydrochloride (9CI) (CA INDEX NAME)



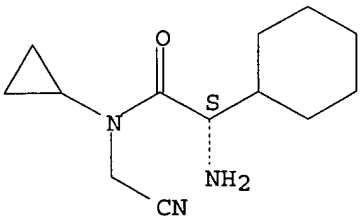
● HCl

RN 848494-00-8 HCAPLUS
CN Acetamide, N-(cyanomethyl)-N-cyclopropyl-2-[(3-hydroxytricyclo[3.3.1.13,7]dec-1-yl)amino]- (9CI) (CA INDEX NAME)



RN 848494-01-9 HCAPLUS
CN Cyclohexaneacetamide, α-amino-N-(cyanomethyl)-N-cyclopropyl-, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

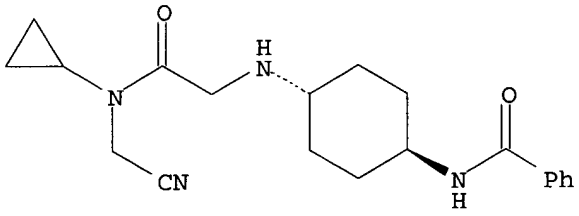
Absolute stereochemistry.



● HCl

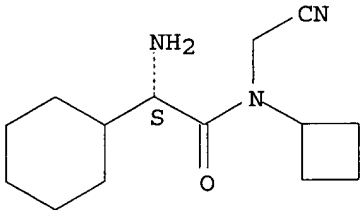
RN 848494-03-1 HCAPLUS
CN Benzamide, N-[trans-4-[[2-[(cyanomethyl)cyclopropylamino]-2-oxoethyl]amino]cyclohexyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 848494-10-0 HCAPLUS
CN Cyclohexaneacetamide, α-amino-N-(cyanomethyl)-N-cyclobutyl-, monohydrochloride, (αS)- (9CI) (CA INDEX NAME)

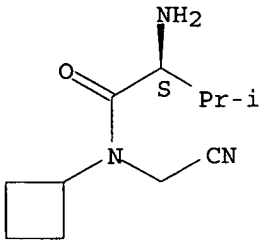
Absolute stereochemistry.



● HCl

RN 848494-11-1 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-N-cyclobutyl-3-methyl-, monohydrochloride, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

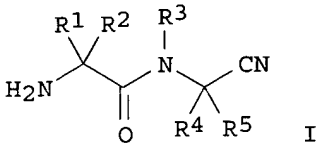
L10 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1127324 HCAPLUS
DOCUMENT NUMBER: 142:56672
TITLE: Preparation of peptidyl nitriles as protease inhibitors
INVENTOR(S): Bondebjerg, Jon; Fuglsang, Henrik; Naerum, Lars
PATENT ASSIGNEE(S): Combio A/S, Den.
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004110988	A1	20041223	WO 2004-DK421	20040617

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:	DK 2003-905	A	20030618
	US 2003-479961P	P	20030619

OTHER SOURCE(S): MARPAT 142:56672
GI



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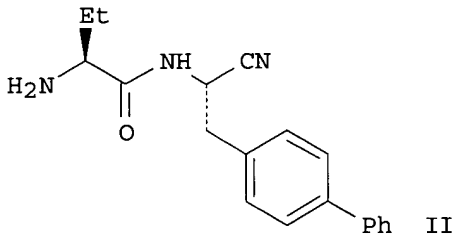


II

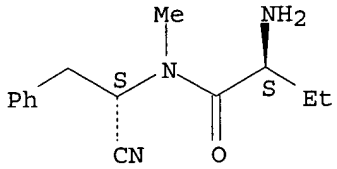
AB Peptidyl nitriles of formula I [R1 = H, alkyl, arylalkyl, etc.; R2, R3, R5 = H, alkyl; R1R2 = (hetero)cycloalkyl; R1R3 = heterocycloalkyl; R4 = H, alkyl, alkoxy, acyl, cycloalkyl, (substituted) arylalkyl, etc.; R4R5 = (hetero)cycloalkyl] are prepared which are capable of selectively inhibiting dipeptidyl-peptidase I (DPP-I), also known as cathepsin C. The compds. are useful for the treatment of inflammation, type 2 **diabetes**, asthma, severe influenza, respiratory syncytial virus infection, CD8 T cell inhibition, inflammatory bowel diseases, psoriasis, atopic dermatitis, Papillon Lefevre syndrome, Haim Munk syndrome, gum disease, periodontitis, rheumatoid arthritis, Huntington's disease, Chagas' disease, Alzheimer's disease, sepsis or for application in target cell apoptosis. Thus, II was prepared, and inhibited DPP-I with IC50 if 13 nM.

IT **810666-06-9P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptidyl nitriles as protease inhibitors)

RN 810666-06-9 HCAPLUS

CN Butanamide, 2-amino-N-[(1S)-1-cyano-2-phenylethyl]-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:1124988 HCAPLUS

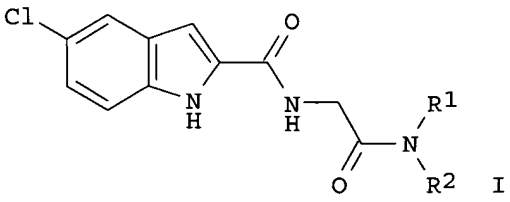
DOCUMENT NUMBER: 142:197810

TITLE: 5-Chloroindoloyl glycine amide inhibitors of glycogen phosphorylase: synthesis, in vitro, in vivo, and X-ray crystallographic characterization

AUTHOR(S): Wright, Stephen W.; Rath, Virginia L.; Genereux, Paul E.; Hageman, David L.; Levy, Carolyn B.; McClure, Lester D.; McCoid, Scott C.; McPherson, R. Kirk; Schelhorn, Teresa M.; Wilder, Donald E.; Zavadoski, William J.; Gibbs, E. Michael; Treadway, Judith L.

CORPORATE SOURCE: Pfizer Global Research and Development, Groton, CT, 06340, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(2), 459-465
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:197810
GI



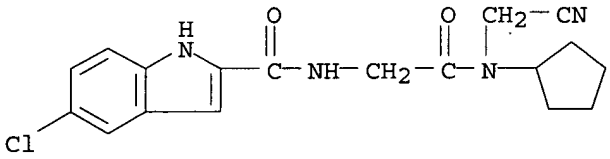
I

AB The synthesis and in vitro and in vivo biol. characterization of a series of achiral 5-chloroindoloyl glycine amides I [R1 = Me, cyclopentyl, HOCH2CH2; R2 = Me2CHCH2, Ph, cycloheptyl, H2N(CH2)3, etc.] as inhibitors of human liver glycogen phosphorylase A are described. Improved potency over previously reported compds. in cellular and in vivo assays was observed The allosteric binding site of these compds. was shown by X-ray crystallog. to be the same as that reported previously for 5-chloroindoloyl norstatine amides.

IT **839701-46-1P**
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of N-carbamoylmethyl indolecarboxamides as human liver glycogen phosphorylase inhibitors)

RN 839701-46-1 HCAPLUS

CN 1H-Indole-2-carboxamide, 5-chloro-N-[2-[(cyanomethyl)cyclopentylamino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN applicants

ACCESSION NUMBER: 2004:368874 HCAPLUS
DOCUMENT NUMBER: 140:357672
TITLE: Preparation of glycinenitrile-based inhibitors of dipeptidyl peptidase IV
INVENTOR(S): Magnin, David R.; Hamann, Lawrence G.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004037181	A2	20040506	WO 2003-US33385	20031021
WO 2004037181	A3	20041021		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004259919	A1	20041223	US 2003-690173	20031021
EP 1553937	A2	20050720	EP 2003-774915	20031021
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
PRIORITY APPLN. INFO.:			US 2002-420603P	P 20021023
			WO 2003-US33385	W 20031021

OTHER SOURCE(S): MARPAT 140:357672

AB Glycinenitrile derivs. R4NHCHR3CONR2CHR1CN [R1 is H, alk(en)(yn)yl or (cyclo)alk(en)yl; R2 is (un)substituted alk(en)(yn)yl, (cyclo)alk(en)yl or arylalk(en)(yn)yl; R3 is group given for R2 or cycloalkylalkyl, alkylthioalkyl, arylalkylthioalkyl, (hetero)aryl, heteroarylalkyl, cycloheteroalkyl or cycloheteroalkylalkyl, which may be substituted; R4 is H or can combine with R3 to form a 4- to 5-membered heterocyclic ring] were prepared for use in pharmaceutical compns. for the treatment of **diabetes** and related diseases. Thus, (S)-H2NCH(Ad)CONEtCH2CN was prepared by condensation of (S)-Boc-NHCH(Ad)CO2H (Boc = tert-butoxycarbonyl) with EtNHCH2CN (syntheses given), followed by deprotection using trifluoroacetic acid.

IT **9004-10-8**, Insulin, biological studies
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(**antidiabetic** agent; preparation of glycinenitrile amino acid derivs. as inhibitors of dipeptidyl peptidase IV)

RN 9004-10-8 HCAPLUS
CN Insulin (9CI) (CA INDEX NAME)

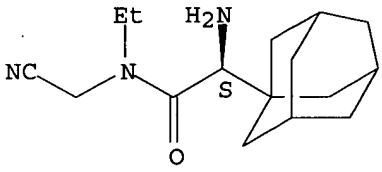
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IT **681282-40-6P 681282-41-7P 681282-42-8P**
681282-43-9P 681282-44-0P 681282-46-2P
681282-47-3P 681282-48-4P 681282-49-5P
681282-50-8P 681282-51-9P 681282-52-0P
681282-53-1P 681282-54-2P 681282-55-3P
681282-56-4P 681282-57-5P 681282-58-6P
681282-59-7P 681282-60-0P 681282-61-1P
681282-62-2P 681282-63-3P 681282-64-4P
681282-65-5P 681282-66-6P 681282-67-7P
681282-79-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of glycinenitrile amino acid derivs. as inhibitors of dipeptidyl peptidase IV)

RN 681282-40-6 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-

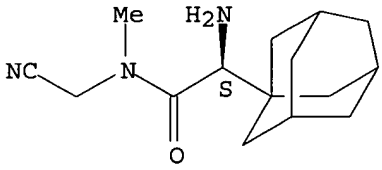
ethyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



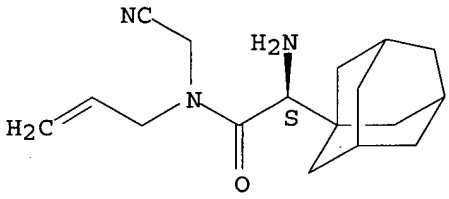
RN 681282-41-7 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



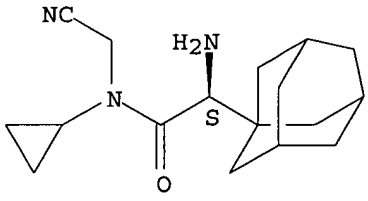
RN 681282-42-8 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-2-propenyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



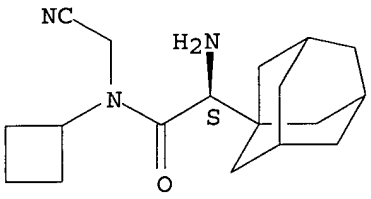
RN 681282-43-9 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-cyclopropyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



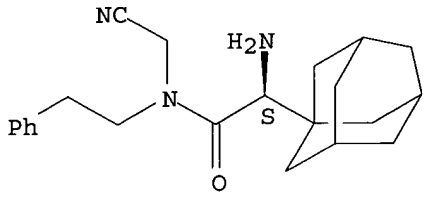
RN 681282-44-0 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-cyclobutyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



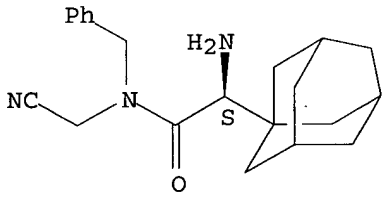
RN 681282-46-2 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-(2-phenylethyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



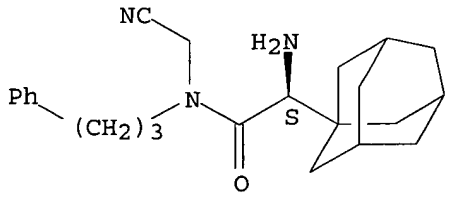
RN 681282-47-3 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-(phenylmethyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



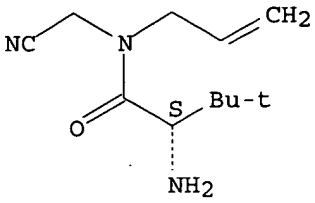
RN 681282-48-4 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-(3-phenylpropyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



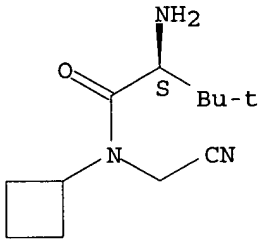
RN 681282-49-5 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-3,3-dimethyl-N-2-propenyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



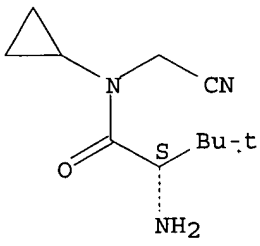
RN 681282-50-8 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-N-cyclobutyl-3,3-dimethyl-, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



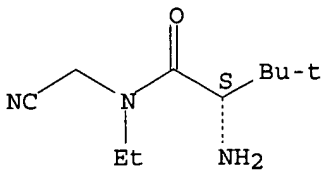
RN 681282-51-9 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-N-cyclopropyl-3,3-dimethyl-, (2S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 681282-52-0 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-N-ethyl-3,3-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

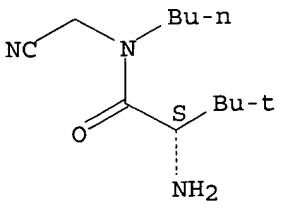
Absolute stereochemistry.



RN 681282-53-1 HCAPLUS

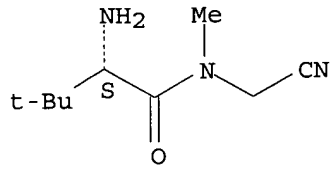
CN Butanamide, 2-amino-N-butyl-N-(cyanomethyl)-3,3-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



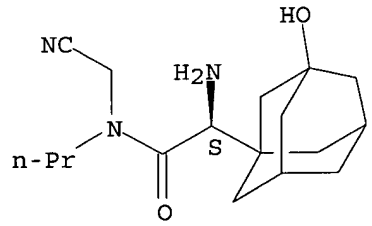
RN 681282-54-2 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-N,3,3-trimethyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



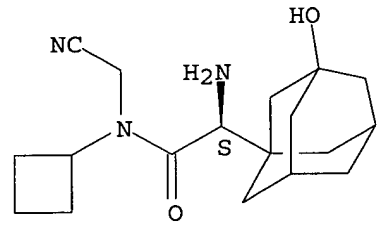
RN 681282-55-3 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-3-hydroxy-N-propyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



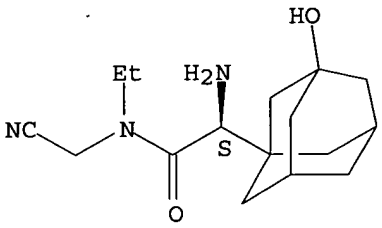
RN 681282-56-4 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-cyclobutyl-3-hydroxy-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



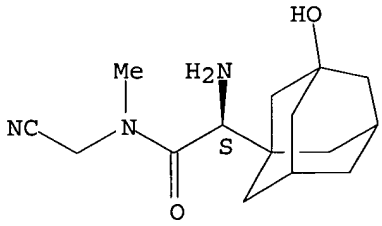
RN 681282-57-5 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-ethyl-3-hydroxy-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



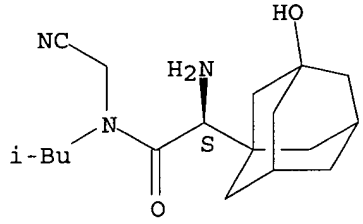
RN 681282-58-6 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-3-hydroxy-N-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



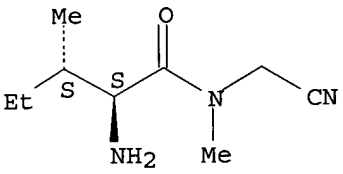
RN 681282-59-7 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-3-hydroxy-N-(2-methylpropyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



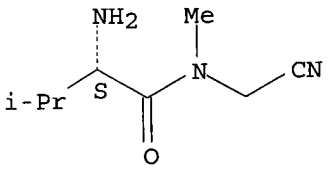
RN 681282-60-0 HCAPLUS
CN Pentanamide, 2-amino-N-(cyanomethyl)-N,3-dimethyl-, (2S,3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



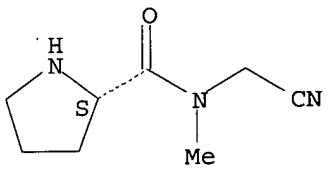
RN 681282-61-1 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-N,3-dimethyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



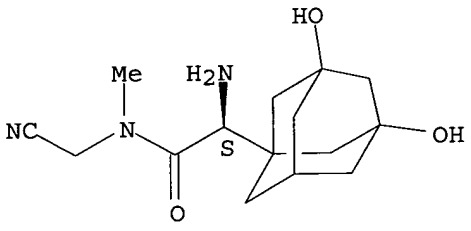
RN 681282-62-2 HCAPLUS
CN 2-Pyrrolidinecarboxamide, N-(cyanomethyl)-N-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



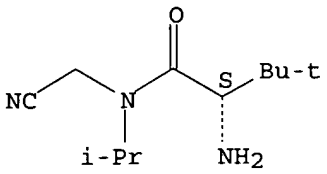
RN 681282-63-3 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-3,5-dihydroxy-N-methyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



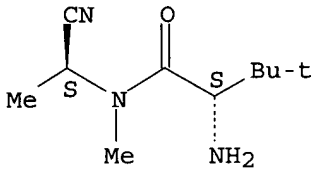
RN 681282-64-4 HCAPLUS
CN Butanamide, 2-amino-N-(cyanomethyl)-3,3-dimethyl-N-(1-methylethyl)-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



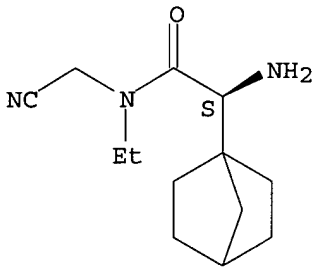
RN 681282-65-5 HCAPLUS
CN Butanamide, 2-amino-N-[(1S)-1-cyanoethyl]-N,3,3-trimethyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



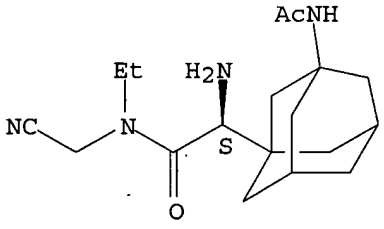
RN 681282-66-6 HCAPLUS
CN Bicyclo[2.2.1]heptane-1-acetamide, α-amino-N-(cyanomethyl)-N-ethyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



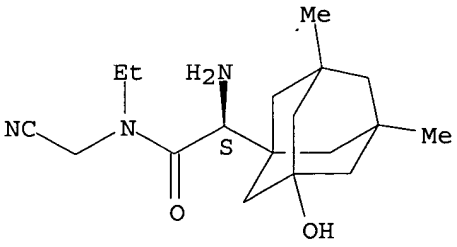
RN 681282-67-7 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, 3-(acetylamino)-α-amino-N-(cyanomethyl)-N-ethyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



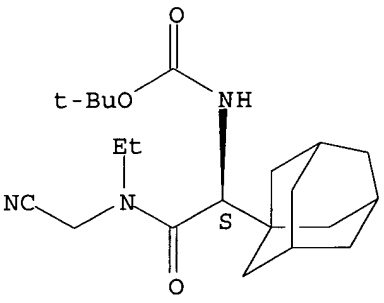
RN 681282-79-1 HCAPLUS
CN Tricyclo[3.3.1.13,7]decane-1-acetamide, α-amino-N-(cyanomethyl)-N-ethyl-3-hydroxy-5,7-dimethyl-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



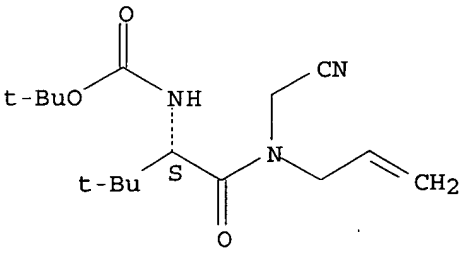
IT **681282-68-8P 681282-69-9P 681282-70-2P**
681282-71-3P 681282-73-5P 681282-74-6P
681282-78-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of glycinenitrile amino acid derivs. as inhibitors of dipeptidyl peptidase IV)
RN 681282-68-8 HCAPLUS
CN Carbamic acid, [(1S)-2-[(cyanomethyl)ethylamino]-2-oxo-1-tricyclo[3.3.1.13,7]dec-1-ylethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 681282-69-9 HCAPLUS
CN Carbamic acid, [(1S)-1-[[(cyanomethyl)-2-propenylamino]carbonyl]-2,2-dimethylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

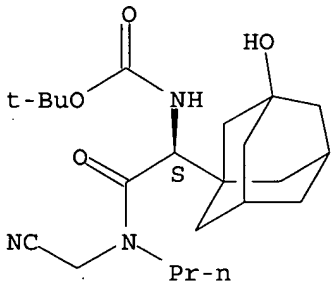
Absolute stereochemistry.



RN 681282-70-2 HCAPLUS
CN Carbamic acid, [(1S)-2-[(cyanomethyl)propylamino]-1-(3-

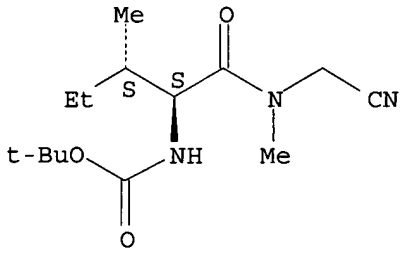
hydroxytricyclo[3.3.1.13,7]dec-1-yl)-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



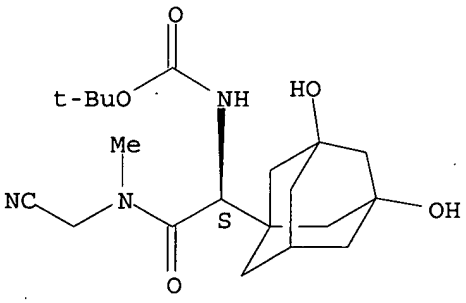
RN 681282-71-3 HCAPLUS
CN Carbamic acid, [(1S,2S)-1-[[(cyanomethyl)methylamino]carbonyl]-2-methylbutyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



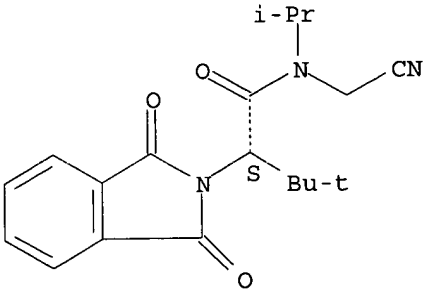
RN 681282-73-5 HCAPLUS
CN Carbamic acid, [(1S)-2-[(cyanomethyl)methylamino]-1-(3,5-dihydroxytricyclo[3.3.1.13,7]dec-1-yl)-2-oxoethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



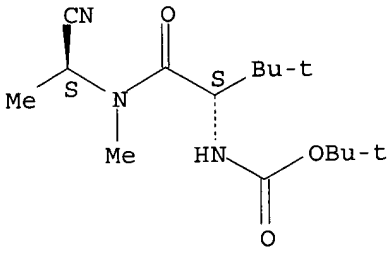
RN 681282-74-6 HCAPLUS
CN 2H-Isoindole-2-acetamide, N-(cyanomethyl)-α-(1,1-dimethylethyl)-1,3-dihydro-N-(1-methylethyl)-1,3-dioxo-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 681282-78-0 HCAPLUS
CN Carbamic acid, [(1S)-1-[[[(1S)-1-cyanoethyl]methylamino]carbonyl]-2,2-dimethylpropyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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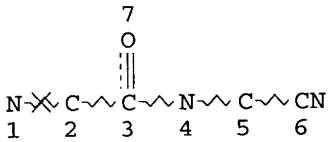
=> d stat que l12
L1 STR



NODE ATTRIBUTES:
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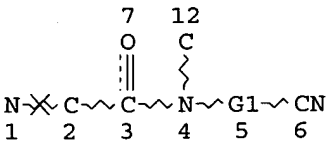
NSPEC IS RC AT 2
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

STEREO ATTRIBUTES: NONE
L5 3934 SEA FILE=REGISTRY SSS FUL L1
L6 STR

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NSPEC   IS RC     AT   2
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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STEREO ATTRIBUTES: NONE
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L9       359971 SEA FILE=HCAPLUS ABB=ON  PLU=ON  DIABETE?/CV OR (HYPERGLYCEMIA/
                CV OR GLUCEMIA/CV OR "GLYCEMIA OR GLUCEMIA"/CV OR "HIGH BLOOD
                GLUCOSE"/CV OR "HIGH BLOOD SUGAR"/CV OR "ANTIDIABETIC AGENTS"/C
                V OR "DIABETES MELLITUS"/CV OR GLUCOSE/CV OR INSULIN/CV) OR
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L10           5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND L9
L11          49 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 NOT L10
L12          37 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND PD=<OCTOBER 23, 2002


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=>

=> d ibib abs hitstr l12 1-37

L12  ANSWER 1 OF 37  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2003:678512  HCAPLUS
DOCUMENT NUMBER:          139:214479
TITLE:                    Preparation of 4-haloalkyl-3-heterocyclylpyridines,
                          4-haloalkyl-5-heterocyclyl-pyrimidines and
                          4-trifluoromethyl-3-oxadiazolylpyridines and their use
                          as pesticides
INVENTOR(S):              Harmsen, Sven; Bastiaans, Henricus Maria Martinus;
                          Schaper, Wolfgang; Tiebes, Jorg; Doller, Uwe; Jans,
                          Daniela; Sanft, Ulrich; Hempel, Waltraud; Thonessen,
                          Maria-theresia; Taapken, Thomas; Rook, Burkhard; Kern,
                          Manfred
PATENT ASSIGNEE(S):       Hoechst Schering Agrevo GmbH, Germany
SOURCE:                   U.S. Pat. Appl. Publ., 90 pp., Cont.-in-part of Ser.
                          No. US 2001-808194, filed on 14 Mar 2001 which is
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   3
PATENT INFORMATION:
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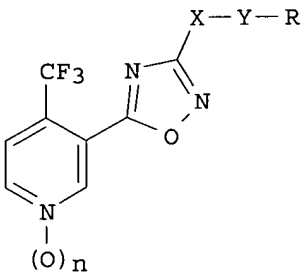
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003162812	A1	20030828	US 2002-56274	20020124
US 6699853	B2	20040302		
DE 19725450	A1	19981217	DE 1997-19725450	19970616 <--
US 6239160	B1	20010529	US 1998-96748	19980612 <--
DE 19858193	A1	20000621	DE 1998-19858193	19981217 <--
US 2002013326	A1	20020131	US 2001-808194	20010314 <--
US 6521610	B2	20030218		

PRIORITY APPLN. INFO.:

DE 1997-19725450	A	19970616
US 1998-96748	A3	19980612
DE 1998-19858193	A	19981217
US 1999-461792	B3	19991215
US 2001-808194	A2	20010314

OTHER SOURCE(S): MARPAT 139:214479

GI



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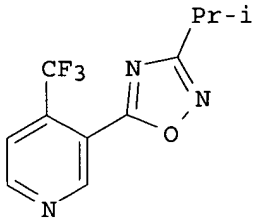


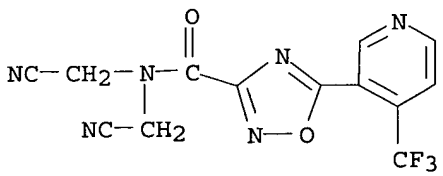
II

AB Title compds. I [n = 0-1; X = bond, (un)branched alkylene; Y = O, S, SO, SO2, OCO, OCO2, etc.; R = H, (cyclo)alk(en/yn)yl, etc.; with provisions] are prepared For instance, Me 4-trifluoromethylnicotinate is reacted with isobutyramide oxime (EtOH, NaOEt, 0°) to give II. Selected examples at 300 ppm effected a mortality of 90-100% on Heliothis virescens. I are useful for controlling animal pests, in particular insects, spider mites, ectoparasites and helminths.

IT **218277-91-9P**
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-haloalkyl-3-heterocyclylpyridines, 4-haloalkyl-5-heterocyclyl-pyrimidines and 4-trifluoromethyl-3-oxadiazolylpyridines and their use as pesticides)

RN 218277-91-9 HCAPLUS

CN 1,2,4-Oxadiazole-3-carboxamide, N,N-bis(cyanomethyl)-5-[4-(trifluoromethyl)-3-pyridinyl]- (9CI) (CA INDEX NAME)



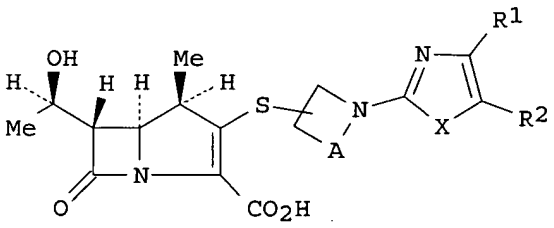
L12 ANSWER 2 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:391717 HCAPLUS
DOCUMENT NUMBER: 136:401574
TITLE: Preparation of 1-methylcarbapenem derivatives as antimicrobial agents
INVENTOR(S): Kobayashi, Yoshiyuki; Shinozuka, Tsuyoshi; Kanno, Osamu
PATENT ASSIGNEE(S): Sankyo Company, Ltd., Japan
SOURCE: PCT Int. Appl., 649 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002040483	A1	20020523	WO 2001-JP9960	20011114 <--
W: AU, BR, CA, CN, CO, CZ, HU, ID, IL, IN, KR, MX, NO, NZ, PH, PL, RU, SG, SK, US, VN, ZA				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2429346	AA	20020523	CA 2001-2429346	20011114 <--
AU 2002015212	A5	20020527	AU 2002-15212	20011114 <--
EP 1340757	A1	20030903	EP 2001-983800	20011114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
BR 2001015454	A	20030923	BR 2001-15454	20011114
NZ 525934	A	20040924	NZ 2001-525934	20011114
RU 2247725	C2	20050310	RU 2003-114408	20011114
JP 2002212182	A2	20020731	JP 2001-349590	20011115 <--
NO 2003002198	A	20030716	NO 2003-2198	20030515
US 2004014962	A1	20040122	US 2003-439198	20030515
ZA 2003003796	A	20040816	ZA 2003-3796	20030515

PRIORITY APPLN. INFO.:	JP 2000-350063	A	20001116
	WO 2001-JP9960	W	20011114

OTHER SOURCE(S): MARPAT 136:401574
GI



I

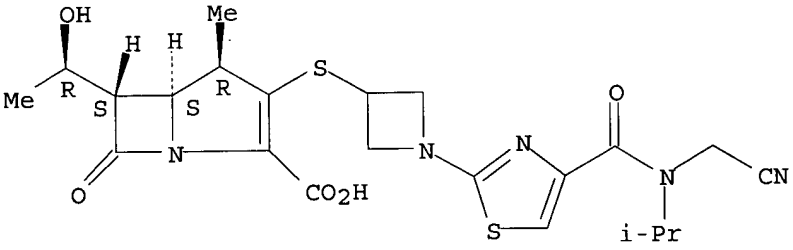
AB The title compds. I [R1 is COOR3 (wherein R3 is hydrogen, C1-6 alkyl, or the like), CONR4R5 (wherein R4 and R5 are each hydrogen, optionally substituted C1-6 alkyl, or the like), cyano, etc.; R2 is hydrogen or C1-6 alkyl; A is (CH2)n; n is 1, 2, or 3; and X is sulfur or oxygen] are prepared Compds. of this invention showed ED50 values of 0.5 mg/kg (s. c.) to 1.7 mg/kg (s. c.) against S. pneumoniae infection in mice. Formulations are given.

IT **429664-34-6P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(preparation of 1-methylcarbapenem derivs. as antimicrobial agents)

RN 429664-34-6 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[1-[4-[[(cyanomethyl)(1-methylethyl)amino]carbonyl]-2-thiazolyl]-3-azetidinyl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, monosodium salt, (4R,5S,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

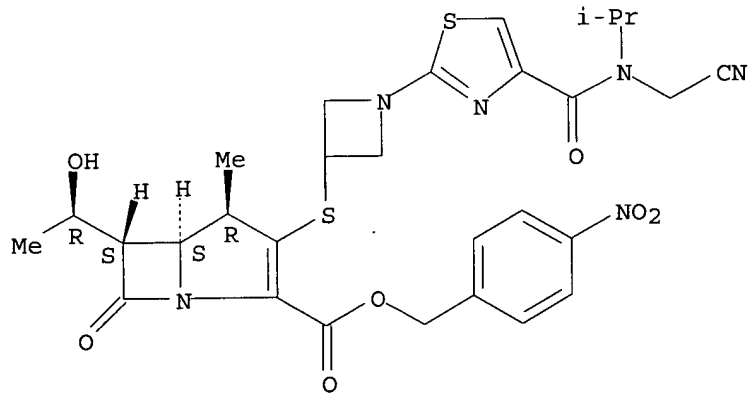


● Na

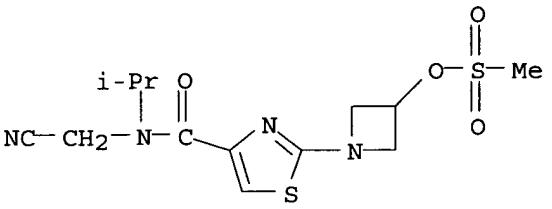
IT **429665-96-3P 429671-13-6P 429671-15-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 1-methylcarbapenem derivs. as antimicrobial agents)

RN 429665-96-3 HCAPLUS
CN 1-Azabicyclo[3.2.0]hept-2-ene-2-carboxylic acid, 3-[[1-[4-[[(cyanomethyl)(1-methylethyl)amino]carbonyl]-2-thiazolyl]-3-azetidinyl]thio]-6-[(1R)-1-hydroxyethyl]-4-methyl-7-oxo-, (4-nitrophenyl)methyl ester, (4R,5S,6S)- (9CI) (CA INDEX NAME)

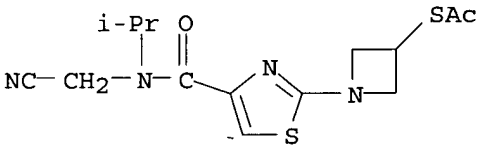
Absolute stereochemistry.



RN 429671-13-6 HCAPLUS
CN 4-Thiazolecarboxamide, N-(cyanomethyl)-N-(1-methylethyl)-2-[3-[(methylsulfonyl)oxy]-1-azetidinyl]- (9CI) (CA INDEX NAME)



RN 429671-15-8 HCAPLUS
CN Ethanethioic acid, S-[1-[4-[[(cyanomethyl)(1-methylethyl)amino]carbonyl]-2-thiazolyl]-3-azetidinyl] ester (9CI) (CA INDEX NAME)

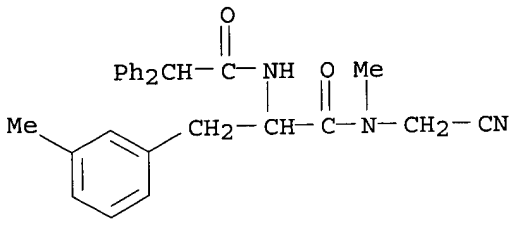


REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 3 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:823645 HCAPLUS
DOCUMENT NUMBER: 136:95585
TITLE: Identification of Dipeptidyl Nitriles as Potent and Selective Inhibitors of Cathepsin B through Structure-Based Drug Design
AUTHOR(S): Greenspan, Paul D.; Clark, Kirk L.; Tommasi, Ruben A.; Cowen, Scott D.; McQuire, Leslie W.; Farley, David L.; van Duzer, John H.; Goldberg, Ronald L.; Zhou, Huanghai; Du, Zhengming; Fitt, John J.; Coppa, David E.; Fang, Zheng; Macchia, William; Zhu, Lijuan; Capparelli, Michael P.; Goldstein, Robert; Wigg, Andrew M.; Doughty, John R.; Bohacek, Regine S.; Knap, Ania K.
CORPORATE SOURCE: Arthritis and Bone Metabolism Research, Novartis Pharmaceuticals Corporation, Summit, NJ, 07901, USA
SOURCE: Journal of Medicinal Chemistry (**2001**), 44(26), 4524-4534
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Cathepsin B is a member of the papain superfamily of cysteine proteases and has been implicated in the pathol. of numerous diseases, including arthritis and cancer. As part of an effort to identify potent, reversible inhibitors of this protease, we examined a series of dipeptidyl nitriles, starting with the previously reported Cbz-Phe-NH-CH2CN (19, IC50 = 62 μM). High-resolution x-ray crystallog. data and mol. modeling were used to optimize the P1, P2, and P3 substituents of this template. Cathepsin B is unique in its class in that it contains a carboxylate recognition site in the S2' pocket of the active site. Inhibitor potency and selectivity were enhanced by tethering a carboxylate functionality from the carbon α to the nitrile to interact with this region of the enzyme. This resulted in the identification of a compound, a 7 nM inhibitor of cathepsin B, with excellent selectivity over other cysteine cathepsins.

IT **389600-08-2P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dipeptidyl nitriles as potent and selective inhibitors of cathepsin B through structure-based drug design)
RN 389600-08-2 HCAPLUS
CN Benzenepropanamide, N-(cyanomethyl)-α-[(diphenylacetyl)amino]-N,3-dimethyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:769282 HCAPLUS
DOCUMENT NUMBER: 135:313616
TITLE: Heterocyclic sulfonyl compounds and activated blood coagulation factor X (FXa) inhibitors containing them
INVENTOR(S): Kobayashi, Shozo; Komoritani, Satoshi; Haginoya, Noriyasu; Suzuki, Masanori; Yoshino, Toshiharu; Nagahara, Takayasu; Yoshikawa, Kenji; Muto, Akira; Ozanai, Takeshi; Nakamoto, Yumi; Mochizuki, Akiyoshi; Nagata, Tsutomu
PATENT ASSIGNEE(S): Daiichi Seiyaku Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 304 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

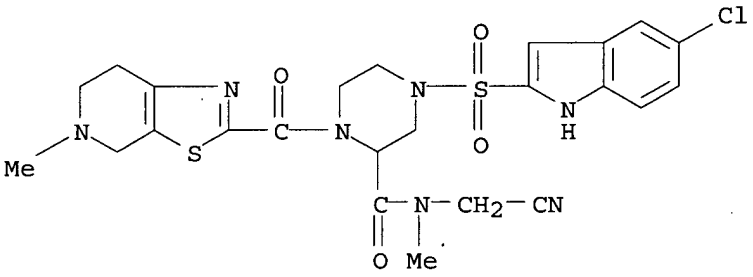
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001294572	A2	20011023	JP 2000-38100	20000209 <--
PRIORITY APPLN. INFO.:			JP 2000-38100	20000209

OTHER SOURCE(S): MARPAT 135:313616
AB Pharmaceuticals, useful for prevention and/or treatment of thrombus and embolus, contain Q1Q2T1SO2QA [I; Q1 = (un)substituted bicyclic or tricyclic group; Q2 = single bond, O, S, C1-6 alkylene, etc.; Q3 = N-containing cyclic group; QA = (un)substituted (hetero)arylalkenyl, bicyclic or tricyclic group, etc.; T1 = CO, (un)substituted methylene, etc.], their salts, or solvates. (2RS)-2-(N-tert-butoxycarbonylaminomethyl)-6-methoxycarbonyl-1,2,3,4-tetrahydronaphthalene was treated with NaOH, condensed with 1-[(6-chloronaphthalen-2-yl)sulfonyl]piperazine.HCl, and deprotected to give (RS)-I.HCl (Q1 = 6-aminomethyl-5,6,7,8-tetrahydronaphthalen-2-yl, Q2 = bond, T1 = CO, Q3 = 1,4-piperazinediyl, QA = 6-chloronaphthalen-2-yl). I.HCl (Q1 = 5-methyl-4,5,6,7-tetrahydrothiazolo[5,4-c]pyridin-2-yl, Q2 = bond, T1 = CO, Q3 = 1,4-piperazinediyl, QA = 6-chloronaphthalen-2-yl) in vitro inhibited human

FXa with IC50 of 20 nM.

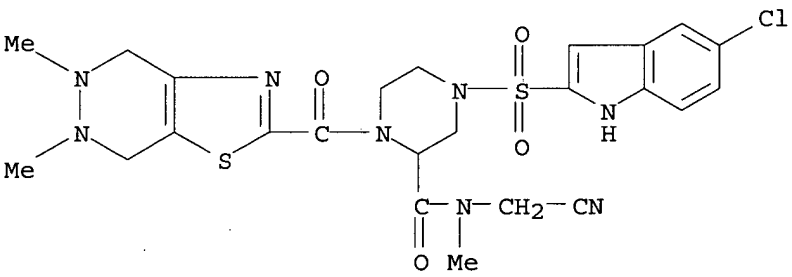
IT **368440-04-4P 368440-75-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of heterocyclic sulfonyl compds. as activated blood coagulation factor X inhibitors)

RN 368440-04-4 HCAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-(cyanomethyl)-N-methyl-1-[(4,5,6,7-tetrahydro-5-methylthiazolo[5,4-c]pyridin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 368440-75-9 HCAPLUS
CN 2-Piperazinecarboxamide, 4-[(5-chloro-1H-indol-2-yl)sulfonyl]-N-(cyanomethyl)-N-methyl-1-[(4,5,6,7-tetrahydro-5,6-dimethylthiazolo[4,5-d]pyridazin-2-yl)carbonyl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L12 ANSWER 5 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:693319 HCAPLUS
DOCUMENT NUMBER: 135:257468
TITLE: Preparation of N-(4-thiazolylbenzoyl)-N-(cyanomethyl)-L-leucinamides and analogs as protease inhibitors
INVENTOR(S): Palmer, James T.; Setti, Eduardo L.; Tian, Zong-Qiang; Venkatraman, Shankar; Wang, Dan-Xiong
PATENT ASSIGNEE(S): Axys Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 73 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

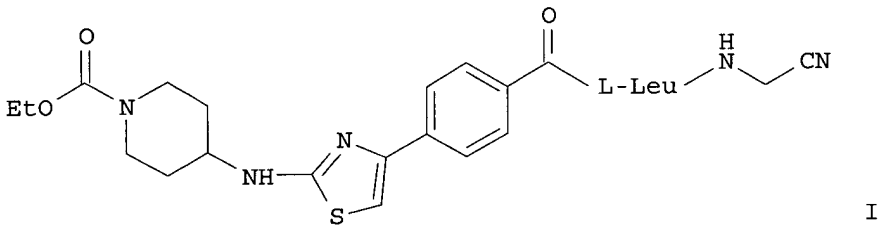
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001068645	A2	20010920	WO 2001-US8332	20010314 <--
WO 2001068645	A3	20020307		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2000-189694P P 20000315

GI



I

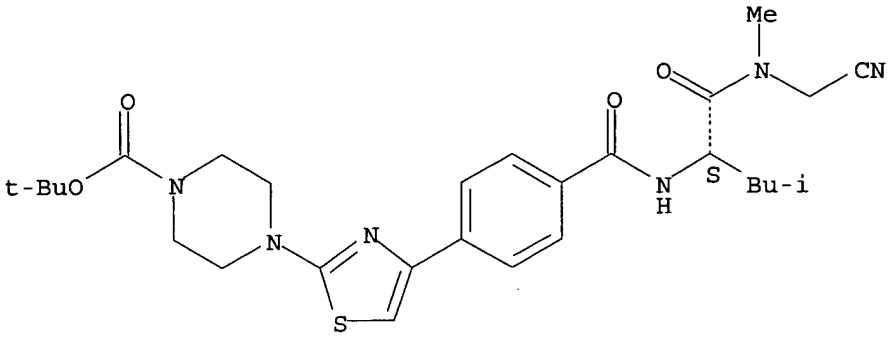
AB The title compds. and their pharmaceutically acceptable salts, N-oxides, prodrugs, protected derivs., or isomers thereof were prepared as cysteine protease inhibitors. For example, stirring a solution of 4-[2-(1-tert-butoxycarbonylpiperidin-4-ylamino)thiazol-4-yl]benzoic acid (preparation given) and the MeSO3H salt of 2S-amino-N-cyanomethyl-4-methylpentanamide overnight at room temperature with PyBOP and diisopropylethylamine in DMF, followed by conversion to the Et ester, yielded I (77%). Test compds. inhibited cathepsin B, K, L, and S (no data). The invention compds. and compns. with a bisphosphonic acid and/or an estrogen receptor agonist are claimed for treating osteoporosis in post-menopausal women (no data).

IT **294622-95-0P 294622-96-1P 294623-08-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-thiazolylbenzoyl-N-cyanomethyl-L-leucinamides and analogs as cysteine protease inhibitors for treatment of osteoporosis)

RN 294622-95-0 HCAPLUS

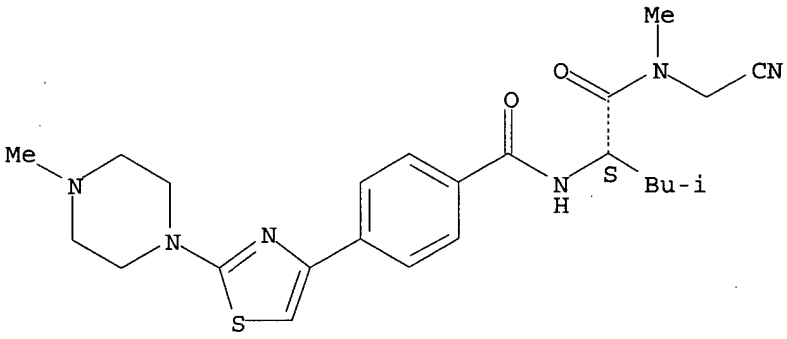
CN 1-Piperazinecarboxylic acid, 4-[4-[4-[[[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]amino]carbonyl]phenyl]-2-thiazolyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



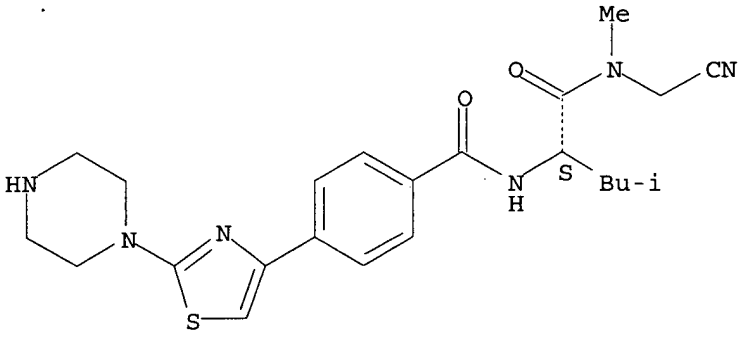
RN 294622-96-1 HCAPLUS
CN Benzamide, N-[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]-4-[2-(4-methyl-1-piperazinyl)-4-thiazolyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 294623-08-8 HCAPLUS
CN Benzamide, N-[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]-4-[2-(1-piperazinyl)-4-thiazolyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 6 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:463222 HCAPLUS
DOCUMENT NUMBER: 135:61327
TITLE: Preparation of pyrazolecarboxylic acid amides and

insecticides and acaricides containing them

INVENTOR(S): Okada, Itaru; Ikeda, Yoshiya; Shiga, Yasushi; Fukuchi, Toshiki

PATENT ASSIGNEE(S): Mitsubishi Chemical Corp., Japan

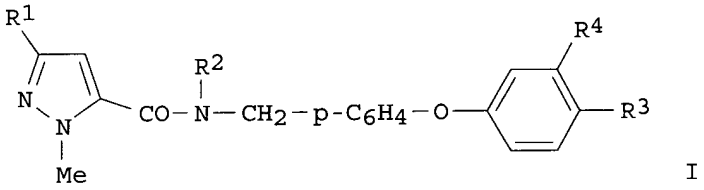
SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001172261	A2	20010626	JP 1999-360588	19991220 <--

PRIORITY APPLN. INFO.: JP 1999-360588 19991220
OTHER SOURCE(S): MARPAT 135:61327

GI



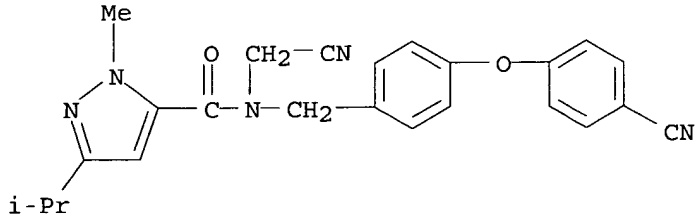
I

AB Title compds. I (R1 = C1-3 (cyclo)alkyl, C1-4 alkoxy, F3C; R2 = C2-5 acyl, C2-10 oxoacyl, C2-10 alkoxycarbonyl, PhOCO, etc.; R3 = H, cyano, C1-4 alkylthio, C1-4 alkylsulfinyl, etc.; R4 = H, C1-4 alkyl) are prepared N-[4-(4-trifluoromethylphenoxy)benzyl]-3-ethyl-1-methylpyrazole-5-carboxylic acid amide (1.0 g) was reacted with acetyl chloride in the presence of NaH in N-methylpyrrolidone at room temperature for 30 min to give 0.51 g I (R1 = Et, R2 = COMe, R3 = CF3, R4 = H) showing 100% acaricide activity.

IT **345289-89-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrazolecarboxylic acid amides and insecticides and acaricides containing them)

RN 345289-89-6 HCAPLUS

CN 1H-Pyrazole-5-carboxamide, N-(cyanomethyl)-N-[[4-(4-cyanophenoxy)phenyl]methyl]-1-methyl-3-(1-methylethyl)- (9CI) (CA INDEX NAME)



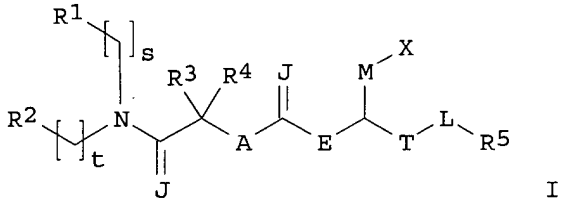
L12 ANSWER 7 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:145268 HCAPLUS
DOCUMENT NUMBER: 134:193742
TITLE: Synthesis of N,N-disubstituted peptide amides for selectively inhibiting the binding of α4β1 integrin
INVENTOR(S): Biediger, Ronald J.; Grabbe, Vanessa O.; Holland, George W.; Kassir, Jamal M.; Kogan, Timothy P.; Lin, Shuqun; Market, Robert V.; Raju, Bore G.; Scott, Ian L.; Wu, Chengde
PATENT ASSIGNEE(S): Texas Biotechnology Corporation, USA
SOURCE: U.S., 30 pp., Cont.-in-part of U.S. Ser. No. 292,187.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6194448	B1	20010227	US 1999-417857	19991014 <--
AU 759154	B2	20030410	AU 2000-66602	20001018
AU 763115	B2	20030710	AU 2000-66601	20001018

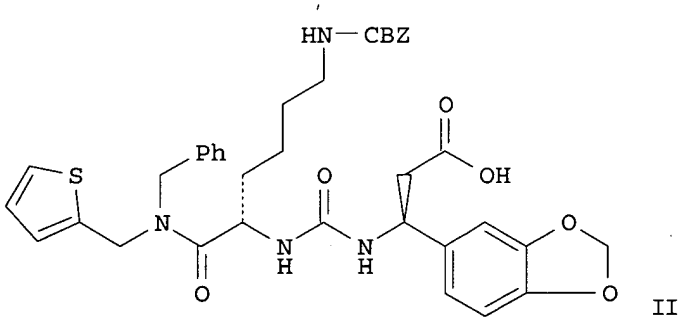
PRIORITY APPLN. INFO.:

US 1998-82019P	P	19980416
US 1999-292187	A2	19990415
AU 1999-35637	A3	19990415
AU 1999-37483	A3	19990415

OTHER SOURCE(S): MARPAT 134:193742
GI



I



II

AB Peptide amides I [A, J = O, S, or (un)substituted amino; E = CH2, O, S, or (un)substituted amino; s, t = 0-3; T = CO, bond, CH2, CH2CH2, or CH2CH2CH2; L = O, S, (un)substituted amino, CH2, or CH2CH2; M = bond or (un)substituted alkylene; X = H, CO2H, carboxy ester, PO3H2, SO3H, OPO3H2,

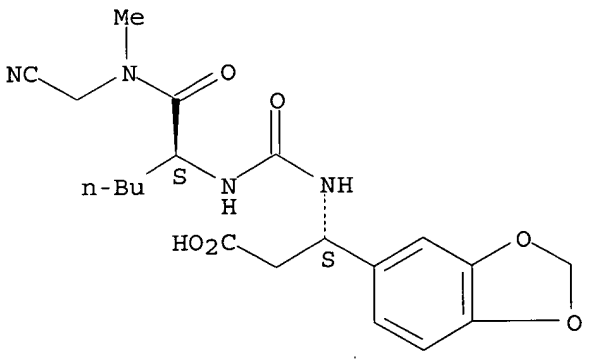
C(O)NHC(O)R12, C(O)NHSO2R13, oxazolyl, tetrazolyl, or H; R1-R5, R12, R13 = H, (cyclo)alkyl, aryl, heterocyclyl, etc.] were prepared as selective inhibitors of the binding of α4β1 integrin to its receptors, such as VCAM-1 (vascular cell adhesion mol.-1) and fibronectin. For example, thiophene-2-methylamine was coupled with benzaldehyde and the product used to amidate Boc-L-Lys(Cbz)-OH (Boc = tert-butoxycarbonyl, Cbz = benzyloxycarbonyl). Deprotection and acylation of the α-amine with (S)-Me 3-[[(p-nitrophenoxy)carbonyl]amino]-3-(1,3-benzodioxol-5-yl)propionate and deesterification yielded peptide II. Invention compds. were assayed for their ability to suppress binding using a 26-amino acid peptide containing the CS-1 sequence of fibronectin with N-terminal cysteine coupled to maleimide activated ovalbumin. Sixty of the test compds. inhibited cell adhesion by 99-100% at concns. of 100 μM and gave IC50 values ranging from 0.0004 to 40.

IT **327035-98-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N,N-disubstituted peptide amides for selectively inhibiting the binding of α4β1 integrin)

RN 327035-98-3 HCAPLUS

CN 1,3-Benzodioxole-5-propanoic acid, β-[[[[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]pentyl]amino]carbonyl]amino]-, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

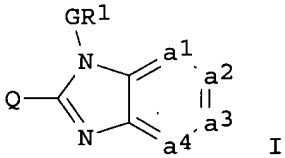
L12 ANSWER 8 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:12448 HCAPLUS
DOCUMENT NUMBER: 134:86251
TITLE: Preparation of benzimidazoles as respiratory syncytial virus replication inhibitors.
INVENTOR(S): Janssens, Frans Eduard; Lacrampe, Jean Fernand Armand; Guillemont, Jerome Emile Georges; Venet, Marc Gaston; Andries, Koenraad Jozef Lodenwijk Marcel
PATENT ASSIGNEE(S): Janssen Pharmaceutica N.V., Belg.
SOURCE: PCT Int. Appl., 102 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001000615	A1	20010104	WO 2000-EP5677	20000620 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2376785	AA	20010104	CA 2000-2376785	20000620 <--
BR 2000011997	A	20020305	BR 2000-11997	20000620 <--
EP 1196410	A1	20020417	EP 2000-936899	20000620 <--
EP 1196410	B1	20040218		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
TR 200103805	T2	20020621	TR 2001-200103805	20000620 <--
JP 2003503403	T2	20030128	JP 2001-507023	20000620
EE 200100694	A	20030217	EE 2001-694	20000620
AT 259796	E	20040315	AT 2000-936899	20000620
EP 1400519	A1	20040324	EP 2003-102464	20000620
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
NZ 515392	A	20040326	NZ 2000-515392	20000620
AU 774829	B2	20040708	AU 2000-52222	20000620
PT 1196410	T	20040730	PT 2000-936899	20000620
ES 2215670	T3	20041016	ES 2000-936899	20000620
TR 200500707	T2	20050421	TR 2005-200500707	20000620
HR 2001000934	A1	20030630	HR 2001-934	20011219
ZA 2001010473	A	20030320	ZA 2001-10473	20011220
NO 2001006370	A	20011227	NO 2001-6370	20011227 <--
BG 106288	A	20021031	BG 2002-106288	20020108
HK 1045998	A1	20050603	HK 2002-107623	20021021
PRIORITY APPLN. INFO.:			EP 1999-202089 A	19990628
			EP 2000-936899 A3	20000620
			WO 2000-EP5677 W	20000620

OTHER SOURCE(S): MARPAT 134:86251

GI



I

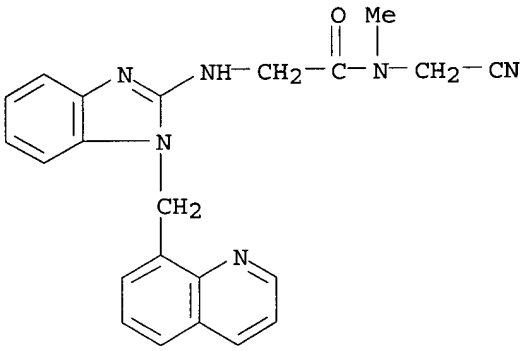
AB Title compds. [I; a1:a2a3:a4 = (substituted) CH:CHCH:CH, N:CHCH:CH, CH:NCH:CH; CH:CHN:CH, CH:CHCH:N; Q = R2R4NAX1, R2R4NCOAX1, specified (substituted) (hetero)cycles; A = (substituted) alkylene; X1 = imino, S, SO, SO2, O, CH2, CO, CH(OH), etc.; R1 = (substituted) bicyclic heterocycle; G = bond, (substituted) alkylene; R2 = H, CHO, alkylcarbonyl, pyrrolidinyl, piperidinyl, homopiperidinyl, etc.; R4 = H, alkyl, aralkyl], were prepared Thus, 1-[4-[[1-(2-quinolylmethyl)-1H-benzimidazol-2-yl]amino]-1-piperidinyl]-3-methyl-2-butanone was hydrogenated with PhCH2NH2 in MeOH

over Pd/C to give N-[1-(2-amino-3-methylbutyl)-4-piperidinyl]-1-(2-quinolylmethyl)-1H-benzimidazol-2-amine and N-[1-(2-amino-3-methylbutyl)-4-piperidinyl]-1-[(1,2,3,4-tetrahydro-2-quinolyl)methyl]-1H-benzimidazol-2-amine tetrahydrochloride. Tested I inhibited respiratory syncytial virus replication with IC50 = 0.0004-1.5849 μM.

IT **317594-86-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzimidazoles as respiratory syncytial virus replication inhibitors)

RN 317594-86-8 HCAPLUS

CN Acetamide, N-(cyanomethyl)-N-methyl-2-[[1-(8-quinolinylmethyl)-1H-benzimidazol-2-yl]amino]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:666701 HCAPLUS
DOCUMENT NUMBER: 133:252050
TITLE: Preparation of novel N-cyanomethyl amide compounds and compositions as protease inhibitors to treat osteoporosis
INVENTOR(S): Bryant, Clifford M.; Palmer, James T.; Rydzewski, Robert M.; Setti, Eduardo L.; Tian, Zong-Qiang; Venkatraman, Shankar; Wang, Dan-Xiong
PATENT ASSIGNEE(S): Axys Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 155 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000055126	A2	20000921	WO 2000-US6837	20000315 <--
WO 2000055126	A3	20010222		

W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE,

DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

CA 2368148	AA	20000921	CA 2000-2368148	20000315 <--
EP 1161415	A2	20011212	EP 2000-916375	20000315 <--
EP 1161415	B1	20050713		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO

BR 2000009043	A	20020108	BR 2000-9043	20000315 <--
TR 200103337	T2	20020321	TR 2001-200103337	20000315 <--
TR 200103390	T2	20020521	TR 2001-200103390	20000315 <--
US 6455502	B1	20020924	US 2000-526090	20000315 <--
TR 200201874	T2	20021021	TR 2002-200201874	20000315 <--
US 6476026	B1	20021105	US 2000-526485	20000315
JP 2002539192	T2	20021119	JP 2000-605557	20000315
EE 200100487	A	20030217	EE 2001-487	20000315
AU 769736	B2	20040205	AU 2000-37486	20000315
PT 1178958	T	20040730	PT 2000-916343	20000315
EP 1452522	A2	20040901	EP 2004-75486	20000315
EP 1452522	A3	20050209		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, LT, LV, FI, MK, CY, AL

ES 2215626	T3	20041016	ES 2000-916343	20000315
AT 299493	E	20050715	AT 2000-916375	20000315
ZA 2001007494	A	20020911	ZA 2001-7494	20010911 <--
ZA 2001007495	A	20020911	ZA 2001-7495	20010911 <--
NO 2001004484	A	20011026	NO 2001-4484	20010914 <--
BG 106013	A	20020531	BG 2001-106013	20011012 <--
HR 2001000737	A1	20021031	HR 2001-737	20011012
US 2002086996	A1	20020704	US 2001-17851	20011214 <--
US 6593327	B2	20030715		
US 2003096796	A1	20030522	US 2002-205600	20020724
US 2003119788	A1	20030626	US 2002-241001	20020909
US 2004147745	A1	20040729	US 2004-758893	20040115

PRIORITY APPLN. INFO.:	US 1999-124420P	P 19990315
	EP 2000-916343	A3 20000315
	US 2000-526090	A1 20000315
	US 2000-526485	A3 20000315
	WO 2000-US6837	W 20000315
	US 2002-205600	B1 20020724

OTHER SOURCE(S): MARPAT 133:252050

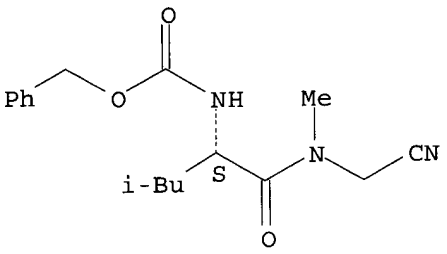
AB Title compds. [R1R2NCR3R4CN; R1 = R11R7NCR5R9X1, R11R8NCR6R10X2NR7CR5R9CX1; X1, X2 independently = CO, CH2SO2; R5, R6 independently = H, C1-6alkyl; R7, R8 independently = H, C1-6alkyl; R9, R10 independently = (un)substituted-C1-6alkyl; R9-R7 = trimethylene, tetramethylene, phenylene-1,2-dimethylene; R10-R8 = trimethylene, tetramethylene, phenylene-1,2-dimethylene; R5-R9 = C3-8cycloalkylene, C3-8heterocycloalkylene; R10-R6 = C3-8cycloalkylene, C3-8heterocycloalkylene; R11 = X4X5R18; X4 = CO, COCO, SO2; X5 = bond, O, NH; R18 = C1-6alkyl; R2 = H, C1-6alkyl; R3 = H, C1-6alkyl; R4 = CN, COOH, COOC1-6alkyl; R2-R4 = trimethylene, tetramethylene, phenylene-1,2-dimethylene; R4-R3 = C3-8cycloalkylene, C3-8heterocycloalkylene], N-oxide, prodrug, isomers, pharmaceutically acceptable salts, and composition are prepared as therapeutically effective estrogen receptor agonist. Title compds. are claimed in treating osteoporosis in post-menopausal woman in which cathepsin K activity contributes to the pathol. and symptomatol. of the disease. Thus, the title compound (S)-C6H5CH2OCONHCH(CH2CH(CH3)2)CONHCH2CN was prepared

IT **294620-35-2P 294621-33-3P 294621-34-4P**
294622-95-0P 294622-96-1P 294622-97-2P
294623-08-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of novel N-cyanomethyl amides and compns. as protease inhibitors)

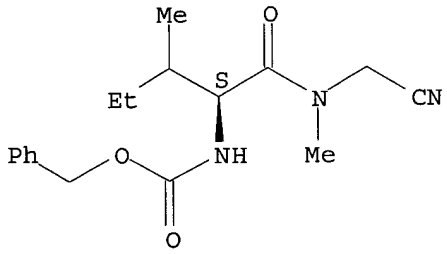
RN 294620-35-2 HCAPLUS
CN Carbamic acid, [(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



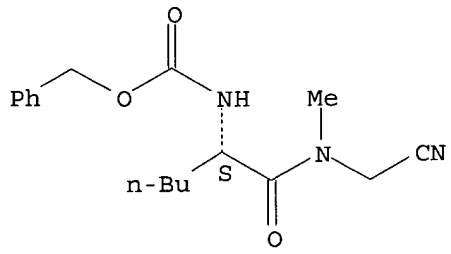
RN 294621-33-3 HCAPLUS
CN Carbamic acid, [(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-2-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



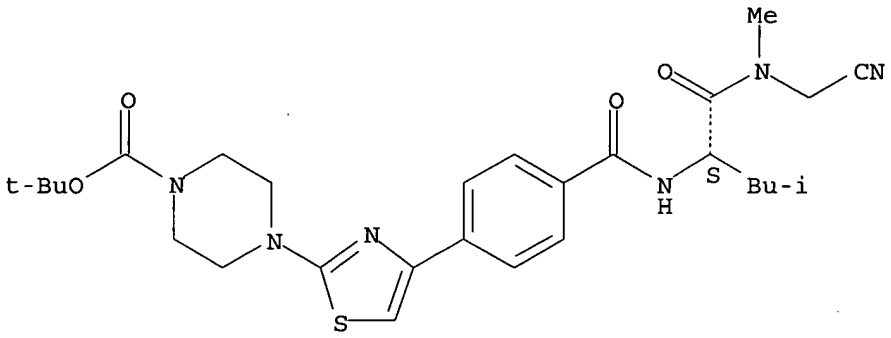
RN 294621-34-4 HCAPLUS
CN Carbamic acid, [(1S)-1-[[(cyanomethyl)methylamino]carbonyl]pentyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



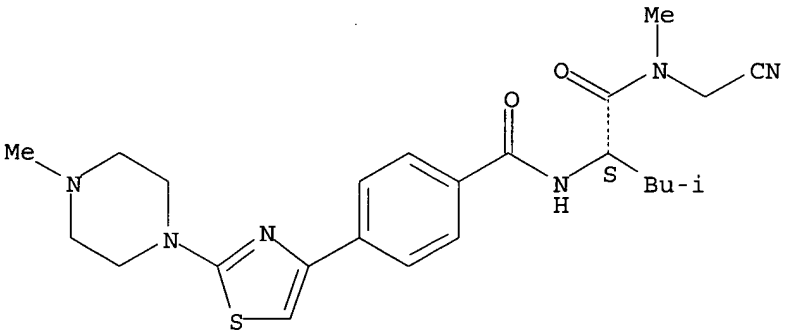
RN 294622-95-0 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[4-[4-[[[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]amino]carbonyl]phenyl]-2-thiazolyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



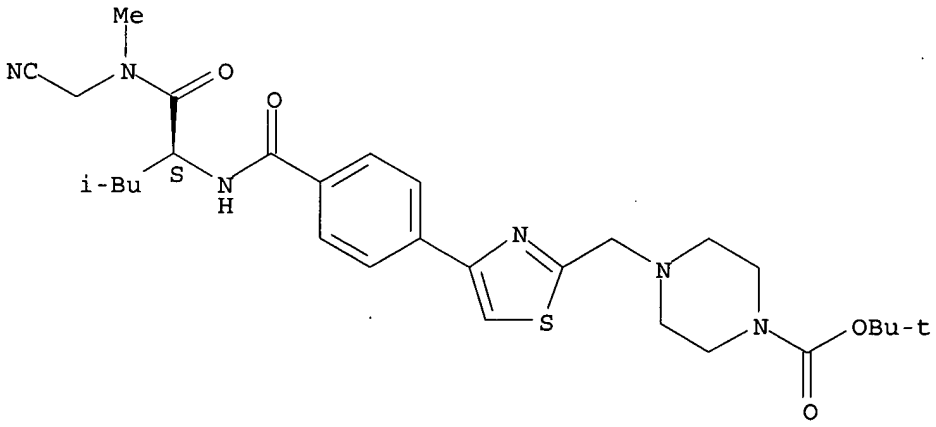
RN 294622-96-1 HCAPLUS
CN Benzamide, N-[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]-4-[2-(4-methyl-1-piperazinyl)-4-thiazolyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



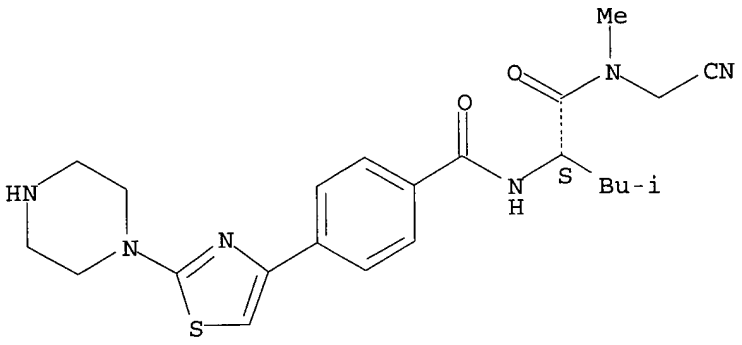
RN 294622-97-2 HCAPLUS
CN 1-Piperazinecarboxylic acid, 4-[[4-[4-[[[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]amino]carbonyl]phenyl]-2-thiazolyl]methyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 294623-08-8 HCAPLUS
CN Benzamide, N-[(1S)-1-[[(cyanomethyl)methylamino]carbonyl]-3-methylbutyl]-4-[2-(1-piperazinyl)-4-thiazolyl]- (9CI) (CA INDEX NAME)

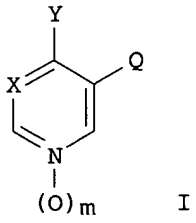
Absolute stereochemistry.



L12 ANSWER 10 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:420911 HCAPLUS
DOCUMENT NUMBER: 133:54868
TITLE: Preparation of 4-haloalkyl-3-heterocyclylpyridines and 4-haloalkyl-5-heterocyclylpyrimidines as repellents
INVENTOR(S): Knauf, Werner; Chapple, Andrew Charles; Wojtech, Eva; Rook, Burkhard
PATENT ASSIGNEE(S): Aventis CropScience GmbH, Germany
SOURCE: PCT Int. Appl., 153 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000035285	A1	20000622	WO 1999-EP9949	19991215 <--
W: AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
DE 19858191	A1	20000621	DE 1998-19858191	19981217 <--
PRIORITY APPLN. INFO.:			DE 1998-19858191 A	19981217

OTHER SOURCE(S): MARPAT 133:54868
GI



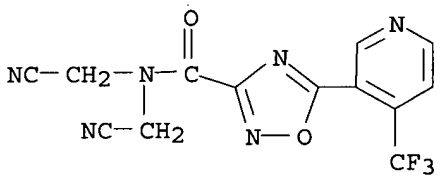
I

AB The title compds. I [Q = (un)substituted 5-membered heterocyclyl; Y = haloalkyl; X = CH or N; m = 0 or 1] are prepared as repellents against insects, spider mites, ectoparasites, helminths, etc.

IT **218277-91-9P 276686-01-2P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation as insect repellent)

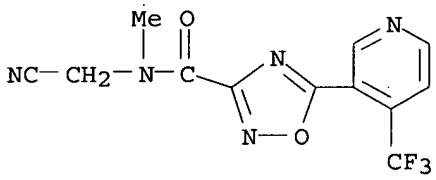
RN 218277-91-9 HCAPLUS

CN 1,2,4-Oxadiazole-3-carboxamide, N,N-bis(cyanomethyl)-5-[4-(trifluoromethyl)-3-pyridinyl]- (9CI) (CA INDEX NAME)



RN 276686-01-2 HCAPLUS

CN 1,2,4-Oxadiazole-3-carboxamide, N-(cyanomethyl)-N-methyl-5-[4-(trifluoromethyl)-3-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:383926 HCAPLUS

DOCUMENT NUMBER: 133:17490

TITLE: Preparation of [1,4]diazepino[2,1-g][1,7]naphthyridine, [1,4]diazonino[2,1-g][1,7]naphthyridine, 13H-[1,4]diazocino[2,1-g][1,7]naphthyridine, and pyrido[3,2-f][1,4]oxazepine derivatives and related compounds as antiemetics

INVENTOR(S): Doi, Takayuki; Yamamoto, Masaki; Fukui, Hideo

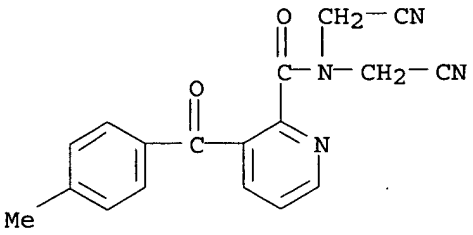
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: PCT Int. Appl., 284 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000032192	A1	20000608	WO 1999-JP6569		19991125 <--
W: AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CR, CU, CZ, DM, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2352612	AA	20000608	CA 1999-2352612		19991125 <--
EP 1145714	A1	20011017	EP 1999-972920		19991125 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2000273042	A2	20001003	JP 1999-336187		19991126 <--
PRIORITY APPLN. INFO.:			JP 1998-337438	A	19981127
			JP 1999-10907	A	19990119
			WO 1999-JP6569	W	19991125

OTHER SOURCE(S): MARPAT 133:17490
GI For diagram(s), see printed CA Issue.
AB Drugs comprising compds. represented by general formula (I) (wherein the ring M is a heterocycle having, as the partial structure X:Y, N:C, CO-N or CS-N; Ra and Rb are bonded to each other to form the ring A, or Ra and Rb are the same or different and each represents hydrogen or a substituent of the ring M; the rings A and B are each an optionally substituted homocyclic or heterocycle and at least one of them is an optionally substituted heterocycle; the ring C is an optionally substituted homocyclic or heterocycle; the ring Z is an optionally substituted nitrogen-containing heterocycle; and n is an integer of 1 to 6) or salts thereof combined with emetic drugs are claimed. The compds. I or salts thereof are useful as antiemetic agents which, in particular, can rapidly and safely inhibit even at a small dose emesis induced by emetic drugs such as anticancer agents, morphine, and apomorphine. Thus, a mixture of (R)-N-[3,5-bis(trifluoromethyl)benzyl]-7,8-dihydro-7-(4-hydroxy-3-methylbutyl)-5-(4-methylphenyl)-8-oxo-6-pyrido[3,4-b]pyridinecarboxamide (preparation given), Et3N, and MeSO2Cl in THF was stirred at room temperature for 30 min, followed by treatment of the product with NaH in THF at room temperature for 1.5 h to give (9R)-7-[3,5-bis(trifluoromethyl)benzyl]-6,7,8,9,10,11-hexahydro-9-methyl-5-(4-methylphenyl)-6,13-dioxo-13H-[1,4]diazocino[2,1-g][1,7]naphthyridine (II). II at 1-10 mg/kg p.o. in vivo inhibited cisplatin-induced emesis in male ferret. Pharmaceutical formulations containing I were prepared
IT **183550-72-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 13H-[1,4]diazocino[g][1,7]naphthyridine derivs. and related compds. as antiemetics)
RN 183550-72-3 HCAPLUS
CN 2-Pyridinecarboxamide, N,N-bis(cyanomethyl)-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

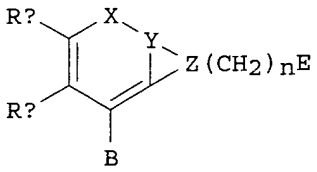
L12 ANSWER 12 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:613656 HCAPLUS
DOCUMENT NUMBER: 131:228734
TITLE: Preparation of diazocinonaphthyridines, diazepinonaphthyridines, and related compounds having tachykinin receptor antagonistic activity for preventing or treating depression, anxiety, manic-depressive illness or psychopathy.
INVENTOR(S): Natsugari, Hideaki; Doi, Takayuki; Ikeura, Yoshinori
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 207 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9947132	A2	19990923	WO 1999-JP1358	19990318 <--
WO 9947132	A3	19991111		
W: AE, AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2321155	AA	19990923	CA 1999-2321155	19990318 <--
AU 9928532	A1	19991011	AU 1999-28532	19990318 <--
AU 751114	B2	20020808		
JP 11322748	A2	19991124	JP 1999-72954	19990318 <--
BR 9908895	A	20001205	BR 1999-8895	19990318 <--
EP 1061926	A2	20001227	EP 1999-909233	19990318 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
EP 1184036	A2	20020306	EP 2001-127194	19990318 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
NO 2000004144	A	20001010	NO 2000-4144	20000818 <--
US 2002132817	A1	20020919	US 2002-97791	20020313 <--

PRIORITY APPLN. INFO.:		
JP 1998-69999	A	19980319
EP 1999-909233	A3	19990318
WO 1999-JP1358	W	19990318
US 1999-308311	A1	19990518

OTHER SOURCE(S): MARPAT 131:228734

GI



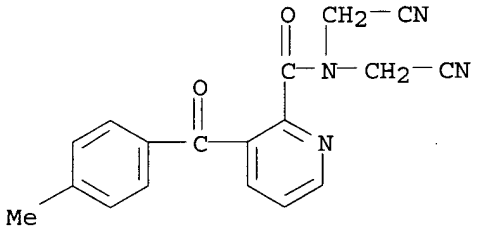
I

AB Pharmaceutical compns. for preventing or treating depression, anxiety, manic-depression, or psychopathy [I; XY = N:C, CON, CSN; Ra, Rb = H, substituent; RaRb = atoms to form a (substituted) (heterocyclic) ring; B, E = (substituted) homocyclic or heterocyclic ring, Z = (substituted) N-containing heterocyclic ring; n = 1-6; with provisos], are claimed. Thus, (9R)-7-[3,5-bis(trifluoromethyl)benzyl]-6,7,8,9,10,11-hexahydro-9-methyl-5-(4-methylphenyl)-6,13-dioxo-13H-[1,4]-diazocino[2,1-g][1,7]naphthyridine (II) (preparation described) antagonized substance P with IC50 = 0.43 nM. A II tablet formulation is given.

IT **183550-72-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of diazocinonaphthyridines, diazepinonaphthyridines, and related compds. having tachykinin receptor antagonistic activity)

RN 183550-72-3 HCAPLUS

CN 2-Pyridinecarboxamide, N,N-bis(cyanomethyl)-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 13 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:9849 HCAPLUS

DOCUMENT NUMBER: 130:66513

TITLE: Preparation of 4-haloalkyl-3-heterocyclylpyridines and 4-haloalkyl-5-heterocyclylpyrimidines as pesticides.

INVENTOR(S): Tiebes, Jorg; Taapken, Thomas; Rook, Burkhard; Kern, Manfred; Sanft, Ulrich

PATENT ASSIGNEE(S): Hoechst Schering Agrevo G.m.b.H., Germany

SOURCE: PCT Int. Appl., 144 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9857969	A1	19981223	WO 1998-EP3321	19980603 <--

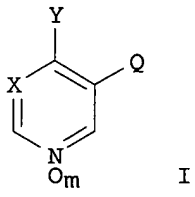
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, GW, HU, ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG

DE 19725450	A1	19981217	DE 1997-19725450	19970616 <--
CA 2294888	AA	19981223	CA 1998-2294888	19980603 <--
AU 9886243	A1	19990104	AU 1998-86243	19980603 <--
AU 754182	B2	20021107		
EP 991648	A1	20000412	EP 1998-937442	19980603 <--
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, PT				
TR 9903102	T2	20000421	TR 1999-9903102	19980603 <--
JP 2002504127	T2	20020205	JP 1999-503659	19980603 <--
CN 1102149	B	20030226	CN 1998-806236	19980603
BR 9810139	A	20000808	BR 1998-10139	19980606 <--
TW 508352	B	20021101	TW 1998-87109414	19980612
ZA 9805180	A	19981217	ZA 1998-5180	19980615 <--

PRIORITY APPLN. INFO.: DE 1997-19725450 A 19970616
WO 1998-EP3321 W 19980603

OTHER SOURCE(S): MARPAT 130:66513

GI



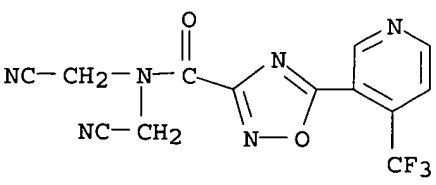
I

AB Title compds. [I; Q = specified (substituted) 5-membered heterocyclyl; Y = haloalkyl; X = CH, N; m = 0, 1], were prepared Thus, Me 4-trifluoromethylnicotinate and isobutyramide oxime were refluxed in EtOH to give 3-isopropyl-5-(4-trifluoromethyl-3-pyridyl)-1,2,4-oxadiazole. The latter at 300 ppm gave 90-100% control of Aphis fabae on beans.

IT **218277-91-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 4-haloalkyl-3-heterocyclylpyridines and 4-haloalkyl-5-heterocyclylpyrimidines as pesticides)

RN 218277-91-9 HCAPLUS

CN 1,2,4-Oxadiazole-3-carboxamide, N,N-bis(cyanomethyl)-5-[4-(trifluoromethyl)-3-pyridinyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

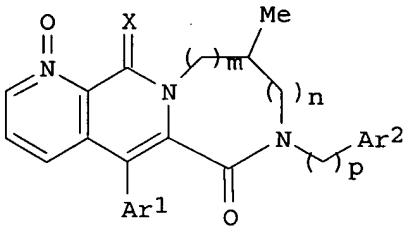
L12 ANSWER 14 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:427772 HCAPLUS
DOCUMENT NUMBER: 129:95515
TITLE: Preparation of medium-ring polycyclic heterocycles as tachykinin receptor antagonists
INVENTOR(S): Natsugari, Hideaki; Ishimaru, Takenori; Doi, Takayuki; Ikeura, Yoshinori; Kimura, Chiharu; Tarui, Naoki
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: U.S., 66 pp., Cont.-in-part of U.S. Ser. No. 621,360.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5770590	A	19980623	US 1996-717801	19960923 <--
JP 09263585	A2	19971007	JP 1996-66337	19960322 <--
JP 2976097	B2	19991110		
JP 09263587	A2	19971007	JP 1997-20386	19960322 <--
CN 1140172	A	19970115	CN 1996-106081	19960323 <--
US 5786352	A	19980728	US 1996-621360	19960325 <--
SG 69968	A1	20000125	SG 1996-6546	19960325 <--
US 6147071	A	20001114	US 1998-87894	19980601 <--
US 6489315	B1	20021203	US 2000-644306	20000823

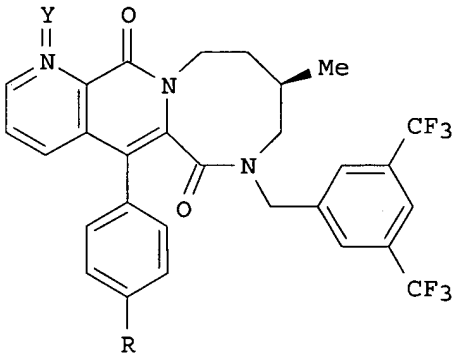
PRIORITY APPLN. INFO.:

JP 1995-91436	A	19950324
JP 1995-207553	A	19950720
JP 1995-264727	A	19950918
JP 1996-30033	A	19960123
JP 1996-66337	A	19960322
US 1996-621360	A2	19960325
JP 1996-214698	A	19960814
US 1998-87894	A3	19980601

OTHER SOURCE(S): MARPAT 129:95515
GI



I



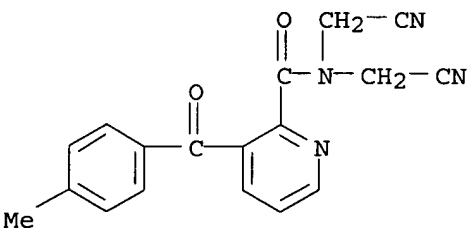
II

AB A variety of polycyclic heterocycles are disclosed, and in particular the compds. I and salts are claimed [wherein X = O, S; Ar1, Ar2 = certain (un)substituted Ph; m, n = 0 to 4; (m+n) = 2 to 4; p = 1 to 6]. The compds. show an excellent tachykinin receptor antagonistic effect. For instance, (9R)-7-[3,5-bis(trifluoromethyl)benzyl]-6,7,8,9,10,11-hexahydro-9-methyl-5-(4-methylphenyl)-6,13-dioxo-13H-[1,4]diazocino[2,1-g][1,7]naphthyridine, i.e., II [Y = absent, R = Me] (preparation given) underwent hydroxylation by Streptomyces subrutilus IFO 13388 to give II [Y = absent, R = CH2OH] (III). The latter underwent acetylation with Ac2O and pyridine, N-oxidation with m-ClC6H4C(O)OOH, and hydrolytic deacetylation, to give title compound II [Y = O, R = CH2OH]. III had an ID50 of 2.5 μg/kg i.v. for inhibiting capsaicin-induced tracheal plasma extravasation in anesthetized guinea pigs. I also showed substance P receptor antagonistic and NK2 receptor inhibitory activities.

IT **183550-72-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of medium-ring polycyclic heterocycles as tachykinin receptor antagonists)

RN 183550-72-3 HCAPLUS

CN 2-Pyridinecarboxamide, N,N-bis(cyanomethyl)-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)

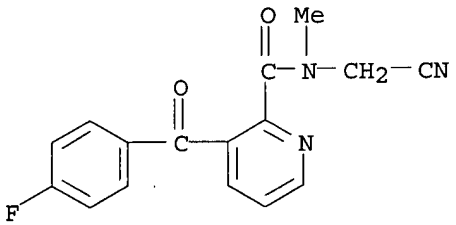


REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

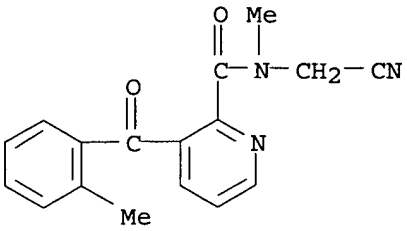
L12 ANSWER 15 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:151429 HCAPLUS
DOCUMENT NUMBER: 126:157495
TITLE: Preparation of pyridopyridine derivatives as tachykinin antagonists
INVENTOR(S): Natsukari, Hideaki; Ishimaru, Takenori; Doi, Takayuki
PATENT ASSIGNEE(S): Takeda Chemical Industries Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 43 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
JP 08337583	A2	19961224	JP 1996-115519		19960412 <--
PRIORITY APPLN. INFO.:			JP 1995-113594	A	19950413

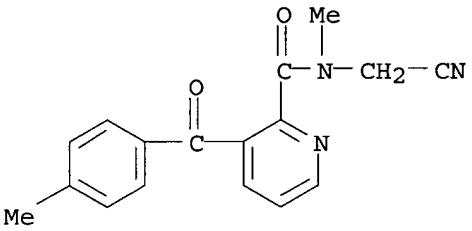
OTHER SOURCE(S): MARPAT 126:157495
GI For diagram(s), see printed CA Issue.
AB The title compds. I [ring A, B = homocyclic ring, heterocyclic ring; at least one of rings A and B is a heterocyclic ring; Z = heterocyclic ring, etc.; R = H, hydrocarbon; one of X and Y is NR1 or O, the other is CO or CS; or one of X and Y is N, the other is CR2; R1 = H, hydrocarbon; R2 = H, halo, etc.; n = 1 - 4], useful as tachykinin antagonists (no data), are prepared For example, 7,8-dihydro-7-methyl-5-(4-methylphenyl)-8-oxo-N-(2-pyridylmethyl)-6-pyrido[3,4-b]pyridinecarboxamide was prepared
IT **168541-96-6P 168542-12-9P 168542-76-5P**
168542-81-2P 168542-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyridopyridine derivs. as tachykinin antagonists)
RN 168541-96-6 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-3-(4-fluorobenzoyl)-N-methyl- (9CI) (CA INDEX NAME)



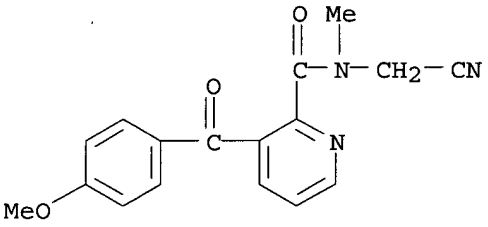
RN 168542-12-9 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-N-methyl-3-(2-methylbenzoyl)- (9CI) (CA INDEX NAME)



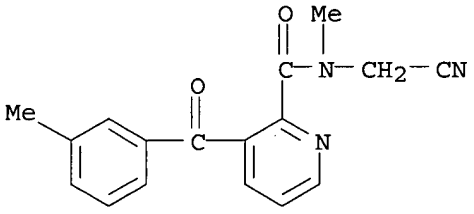
RN 168542-76-5 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-N-methyl-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)



RN 168542-81-2 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-3-(4-methoxybenzoyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 168542-94-7 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-N-methyl-3-(3-methylbenzoyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 16 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:728630 HCAPLUS
DOCUMENT NUMBER: 126:8145

TITLE: Preparation of polycyclic heterocycles as tachykinin receptor antagonists

INVENTOR(S): Natsugari, Hideaki; Ishimaru, Takenori; Doi, Takayuki; Ikeura, Yoshinori; Kimura, Chiharu

PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 94 pp.
CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
EP 733632	A1	19960925	EP 1996-104500		19960321	<--
EP 733632	B1	20030604				
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE						
NO 9601160	A	19960925	NO 1996-1160		19960321	<--
NO 309272	B1	20010108				
TW 394773	B	20000621	TW 1996-85103427		19960321	<--
AT 242243	E	20030615	AT 1996-104500		19960321	
ES 2194937	T3	20031201	ES 1996-104500		19960321	
CA 2172421	AA	19960925	CA 1996-2172421		19960322	<--
AU 9648261	A1	19961003	AU 1996-48261		19960322	<--
AU 699611	B2	19981210				
CN 1140172	A	19970115	CN 1996-106081		19960323	<--
IL 117631	A1	20001121	IL 1996-117631		19960324	<--
BR 9601125	A	19980106	BR 1996-1125		19960325	<--
SG 69968	A1	20000125	SG 1996-6546		19960325	<--
US 6489315	B1	20021203	US 2000-644306		20000823	
PRIORITY APPLN. INFO.:			JP 1995-91436	A	19950324	
			JP 1995-207553	A	19950720	
			JP 1995-264727	A	19950918	
			JP 1996-30033	A	19960123	
			US 1996-621360	A3	19960325	
			US 1998-87894	A3	19980601	

OTHER SOURCE(S): MARPAT 126:8145

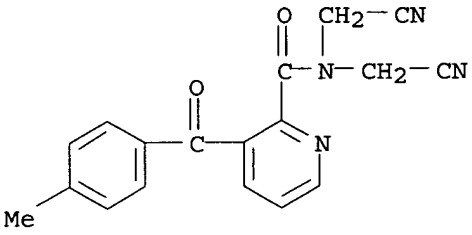
GI For diagram(s), see printed CA Issue.

AB Title compds. [I; R = (CH2)nR4; R1,R2 = H or a substituent; R1R2 = atoms to complete a (hetero)cyclic ring; ring B = heterocyclic ring; R3,R4 = (hetero)cyclic ring; X-Y = N:C, C(O)N, C(S)N; n = 1-6] were prepared Thus, 4-BrC6H4Me was condensed with 2,3-pyridinedicarboxylic acid and the product amidated by HN(CH2CN)2 to give, after cyclization in 5 addnl. steps, 7-[3,5-bis(trifluoromethyl)benzyl]-6,7,8,9-tetrahydro-5-(4-methylphenyl)-6,11-dioxo-11H-pyrazino[2,1-g][1,7]naphthyridine. Data for in vitro biol. activity of selected I were given.

IT **183550-72-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of polycyclic heterocycles as tachykinin receptor antagonists)

RN 183550-72-3 HCAPLUS

CN 2-Pyridinecarboxamide, N,N-bis(cyanomethyl)-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 17 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:835514 HCAPLUS
DOCUMENT NUMBER: 123:256684
TITLE: Preparation of pyridopyridinecarboxamides, thienopyridinecarboxamides, and related compounds as tachykinin antagonists and inhibitors of plasma extravasation.
INVENTOR(S): Natsugari, Hideaki; Ishimaru, Takenori; Doi, Takayuki
PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan
SOURCE: Eur. Pat. Appl., 72 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

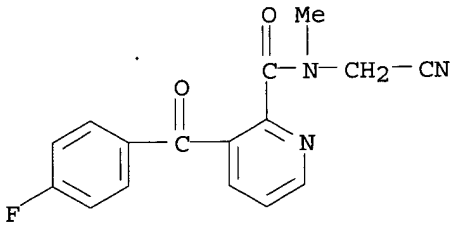
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
EP 652218	A1	19950510	EP 1994-117576		19941108	<--
EP 652218	B1	20010711				
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE						
NO 9404252	A	19950511	NO 1994-4252		19941108	<--
AT 203024	E	20010715	AT 1994-117576		19941108	<--
CA 2135440	AA	19950511	CA 1994-2135440		19941109	<--
FI 9405281	A	19950511	FI 1994-5281		19941109	<--
AU 9477738	A1	19950518	AU 1994-77738		19941109	<--
AU 678295	B2	19970522				
BR 9404403	A	19950718	BR 1994-4403		19941109	<--
JP 08067678	A2	19960312	JP 1994-274699		19941109	<--
RU 2135471	C1	19990827	RU 1994-40174		19941109	<--
HU 68810	A2	19950519	HU 1994-3230		19941110	<--
CN 1107476	A	19950830	CN 1994-113866		19941110	<--
CN 1052004	B	20000503				
US 5585385	A	19961217	US 1994-338762		19941110	<--
BR 9501976	A	19960430	BR 1995-1976		19950509	<--
PRIORITY APPLN. INFO.:			JP 1993-281178	A	19931110	
			JP 1993-337488	A	19931228	
			JP 1994-33637	A	19940303	
			JP 1994-138551	A	19940621	

OTHER SOURCE(S): CASREACT 123:256684; MARPAT 123:256684
GI For diagram(s), see printed CA Issue.
AB Title compds. [I; ring A, ring B = (substituted) homo- or heterocyclyl, ≥1 of them = (substituted) heterocyclyl; ring C = (substituted) benzene ring; R = H, (substituted) hydrocarbyl; 1 of X, Y = NR1, O; the other = CO, CS; or 1 of them = N: and the other = :CR2; R1 = H, (substituted) hydrocarbyl; R2 = H, halo, (substituted) hydrocarbyl, amino, OH; n = 1, 2], were prepared Thus, 5-(4-fluorophenyl)-7,8-dihydro-7-methyl-8-oxo-6-pyrido[3,4-b]pyridinecarboxylic acid (preparation given) was refluxed

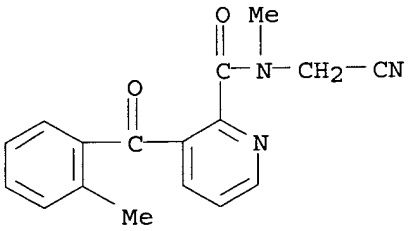
with SOCl2 in benzene and ther residue in THF was refluxed with N-[3,5-bis(trifluoromethyl)benzyl]methylamine and Et3N to give N-[3,5-bis(trifluoromethyl)benzyl]-5-(4-fluorophenyl)-7,8-dihydro-N,7-dimethyl-8-oxo-6-pyrido[3,4-b]pyridinecarboxamide (II). II inhibited substance P binding to IM-9 human lymphoblasts with IC50 = 0.08 nM. Tablets containing II were prepared

IT **168541-96-6P 168542-12-9P 168542-76-5P**
168542-81-2P 168542-94-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyridopyridinecarboxamides, thienopyridinecarboxamides, and related compds. as tachykinin antagonists and inhibitors of plasma extravasation)

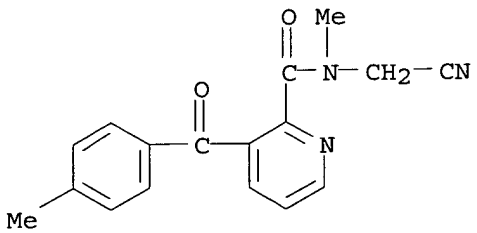
RN 168541-96-6 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-3-(4-fluorobenzoyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 168542-12-9 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-N-methyl-3-(2-methylbenzoyl)- (9CI) (CA INDEX NAME)

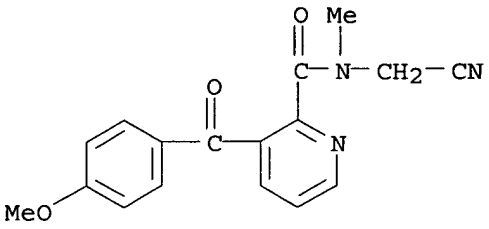


RN 168542-76-5 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-N-methyl-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)

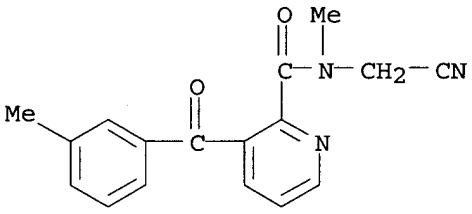


RN 168542-81-2 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-3-(4-methoxybenzoyl)-N-methyl-

(9CI) (CA INDEX NAME)



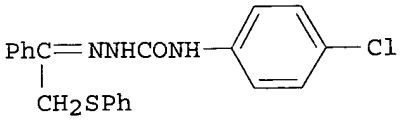
RN 168542-94-7 HCAPLUS
CN 2-Pyridinecarboxamide, N-(cyanomethyl)-N-methyl-3-(3-methylbenzoyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 18 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:735476 HCAPLUS
DOCUMENT NUMBER: 123:169370
TITLE: Preparation of hydrazine-derivative insecticides
INVENTOR(S): Takagi, Kazuhiro; Ohshima, Tetsuji; Hasegawa, Nobuyoshi; Katoh, Chiaki; Kanaoka, Atsushi; Kanno, Hideo
PATENT ASSIGNEE(S): Nihon Nohyaku Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 132 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 657421	A1	19950614	EP 1994-118767	19941129 <--
EP 657421	B1	19990421		
R: CH, DE, ES, FR, GB, IT, LI				
ZA 9409293	A	19950817	ZA 1994-9293	19941123 <--
CA 2136597	AA	19950609	CA 1994-2136597	19941124 <--
CA 2136597	C	20050517		
AU 9479041	A1	19950629	AU 1994-79041	19941125 <--
AU 669458	B2	19960606		
ES 2132310	T3	19990816	ES 1994-118767	19941129 <--
CN 1107142	A	19950823	CN 1994-119875	19941207 <--
CN 1045590	B	19991013		
US 5608109	A	19970304	US 1994-350462	19941207 <--
JP 07215928	A2	19950815	JP 1994-331286	19941208 <--
PRIORITY APPLN. INFO.:			JP 1993-340886 A	19931208

OTHER SOURCE(S): MARPAT 123:169370
GI

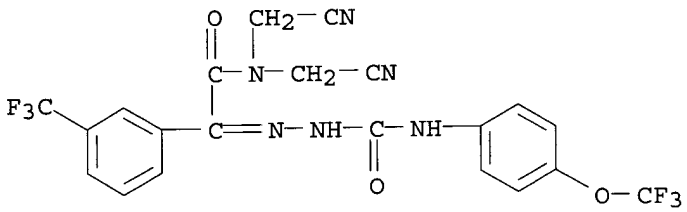


II

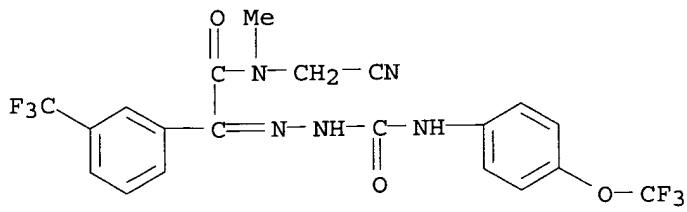
AB The title compds. A1AC(:W)N(A2)R1 [I; A = divalent C:NN or CHNHN radical; A1, A2 = (un)substituted Ph, (un)substituted heteroaryl; R1 = alkyl, etc.], useful as pesticides and insecticides, are prepared and I-cong. formulations presented. Thus, hydrazone derivative II, m.p. 200°, was prepared and demonstrated 100% mortality against Spodoptera litura at 500 ppm.

IT **166309-90-6P 166309-91-7P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of hydrazine-derivative insecticides)

RN 166309-90-6 HCAPLUS
CN Hydrazinecarboxamide, 2-[2-[bis(cyanomethyl)amino]-2-oxo-1-[3-(trifluoromethyl)phenyl]ethylidene]-N-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)



RN 166309-91-7 HCAPLUS
CN Hydrazinecarboxamide, 2-[2-[(cyanomethyl)methylamino]-2-oxo-1-[3-(trifluoromethyl)phenyl]ethylidene]-N-[4-(trifluoromethoxy)phenyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 19 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:699369 HCAPLUS
DOCUMENT NUMBER: 123:340006
TITLE: Novel, Potent, and Orally Active Substance P Antagonists: Synthesis and Antagonist Activity of N-Benzylcarboxamide Derivatives of

Pyrido[3,4-b]pyridine

AUTHOR(S): Natsugari, Hideaki; Ikeura, Yoshinori; Kiyota, Yutaka; Ishichi, Yuji; Ishimaru, Takenori; Saga, Osamu; Shirafuji, Hideo; Tanaka, Toshimasa; Kamo, Izumi; et al.

CORPORATE SOURCE: Pharmaceutical Research Division, Takeda Chemical Industries Ltd., Osaka, 532, Japan

SOURCE: Journal of Medicinal Chemistry (**1995**), 38(16), 3106-20
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

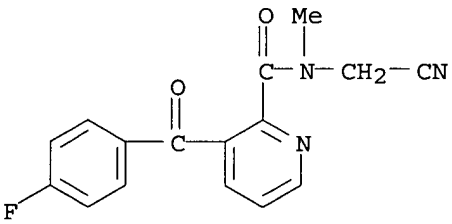
LANGUAGE: English

AB A series of 4-phenylisoquinolone derivs. were synthesized and evaluated for NK1 (substance P) antagonist activity. Highly potent antagonists, 4-phenylisoquinolone-N-benzylcarboxamides, were discovered from the structure-activity relationship studies on N-(1,2-dihydro-2,6,7-trimethyl-1-oxo-4-phenyl-3-isoquinolinyl)-N'-(3-methylphenyl)urea. Optimization of the activity in this series resulted in the development of 5-phenylpyrido[3,4-b]pyridine-N-benzylcarboxamides which are highly potent orally active NK1 antagonists. Among the compds. synthesized, N-[3,5-bis(trifluoromethyl)benzyl]-7,8-dihydro-N,7-dimethyl-8-oxo-5-(substituted phenyl)-6-pyrido[3,4-b]pyridinecarboxamides showed excellent antagonist activities with IC50 values (in vitro inhibition of [125I]BH-SP binding in human IM-9 cells) of 0.21-0.34 nM and ED50 values (in vivo inhibition of capsaicin-induced plasma extravasation in guinea-pig trachea, i.v.) of 0.017-0.030 mg/kg. These compds. exhibited significantly potent activity upon oral administration with ED50 values of 0.068-0.17 mg/kg. Conformational studies on N-[3,5-bis(trifluoromethyl)benzyl]-7,8-dihydro-N,7-dimethyl-8-oxo-5-(substituted phenyl)-6-pyrido[3,4-b]pyridinecarboxamides indicated that the two stable conformers are are quite similar to those of CP-99,994.

IT **168541-96-6P 168542-76-5P 170640-01-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(isoquinolinecarboxamides and pyrido[3,4-b]pyridines as substance P antagonists)

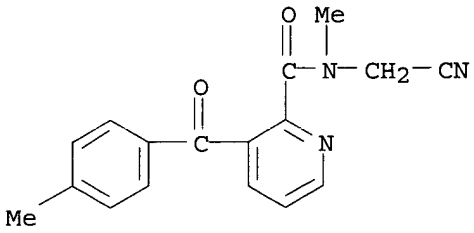
RN 168541-96-6 HCAPLUS

CN 2-Pyridinecarboxamide, N-(cyanomethyl)-3-(4-fluorobenzoyl)-N-methyl- (9CI) (CA INDEX NAME)

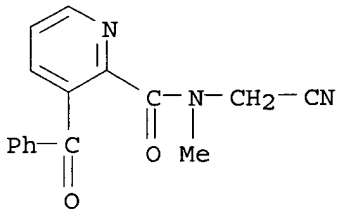


RN 168542-76-5 HCAPLUS

CN 2-Pyridinecarboxamide, N-(cyanomethyl)-N-methyl-3-(4-methylbenzoyl)- (9CI) (CA INDEX NAME)



RN 170640-01-4 HCAPLUS
CN 2-Pyridinecarboxamide, 3-benzoyl-N-(cyanomethyl)-N-methyl- (9CI) (CA INDEX NAME)

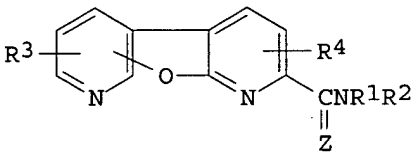


L12 ANSWER 20 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:457335 HCAPLUS
DOCUMENT NUMBER: 121:57335
TITLE: Herbicidal picolinamide derivatives
INVENTOR(S): Bissinger, Hans Joachim; Kleemann, Axel; Searle, Richard John Griffith
PATENT ASSIGNEE(S): "Shell" Research Ltd., S. Afr.
SOURCE: S. African, 78 pp.
CODEN: SFXXAB
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ZA 9206940	A	19930428	ZA 1992-6940	19920911 <--
US 5371061	A	19941206	US 1992-939756	19920902 <--
EP 537816	A1	19930421	EP 1992-202760	19920910 <--
EP 537816	B1	19960424		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 137224	E	19960515	AT 1992-202760	19920910 <--
ES 2087433	T3	19960716	ES 1992-202760	19920910 <--
RO 114614	B1	19990630	RO 1992-1182	19920910 <--
AU 9223543	A1	19930318	AU 1992-23543	19920911 <--
AU 653254	B2	19940922		
CN 1071425	A	19930428	CN 1992-110572	19920911 <--
CN 1042289	B	19990303		
JP 05213882	A2	19930824	JP 1992-267866	19920911 <--
JP 3142392	B2	20010307		
HU 63614	A2	19930928	HU 1992-2915	19920911 <--
HU 218341	B	20000728		
BR 9203528	A	19940301	BR 1992-3528	19920911 <--

RU 2070883	C1	19961227	RU 1992-5052924		19920911 <--
PL 170622	B1	19970131	PL 1992-295912		19920911 <--
PL 170635	B1	19970131	PL 1992-311381		19920911 <--
SK 280305	B6	19991108	SK 1992-2801		19920911 <--
PRIORITY APPLN. INFO.:			EP 1991-115545	A	19910913

OTHER SOURCE(S): MARPAT 121:57335
GI

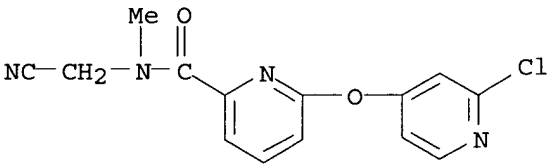


I

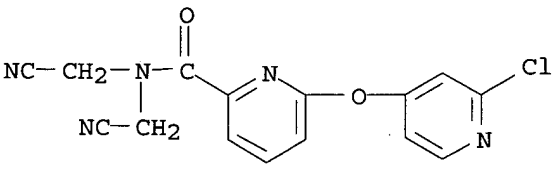
AB The title compds., (pyridinyloxy)picolinamides and (pyridinyloxy)picolinethioamides I (R1, R2 = alkyl, etc.; R3 = hydrogen, halo, alkyl, etc.; R4 = hydrogen, alkyl, halo, etc.; Z = oxygen, sulfur) and their uses as herbicides are claimed.

IT **149527-89-9P 149528-86-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

RN 149527-89-9 HCAPLUS
CN 2-Pyridinecarboxamide, 6-[(2-chloro-4-pyridinyl)oxy]-N-(cyanomethyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 149528-86-9 HCAPLUS
CN 2-Pyridinecarboxamide, 6-[(2-chloro-4-pyridinyl)oxy]-N,N-bis(cyanomethyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 21 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

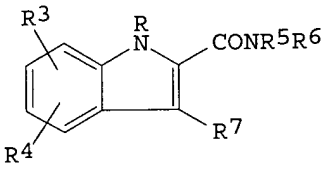
ACCESSION NUMBER:	1994:270104 HCAPLUS
DOCUMENT NUMBER:	120:270104
TITLE:	Preparation of fungicidal indole derivatives
INVENTOR(S):	Curtze, Juergen; Albert, Guido
PATENT ASSIGNEE(S):	Shell Internationale Research Maatschappij B. V.,

Neth.
SOURCE: PCT Int. Appl., 36 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9325524	A1	19931223	WO 1993-EP1406	19930603 <--
W: AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
ZA 9303846	A	19931228	ZA 1993-3846	19930602 <--
AU 9343226	A1	19940104	AU 1993-43226	19930603 <--
AU 666558	B2	19960215		
US 5399559	A	19950321	US 1993-71894	19930603 <--
EP 643695	A1	19950322	EP 1993-912878	19930603 <--
EP 643695	B1	19960814		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 07507323	T2	19950810	JP 1993-501089	19930603 <--
HU 69737	A2	19950928	HU 1994-3475	19930603 <--
HU 216814	B	19990830		
AT 141260	E	19960815	AT 1993-912878	19930603 <--
ES 2091615	T3	19961101	ES 1993-912878	19930603 <--
MD 1743	B2	20010930	MD 1996-960305	19930603 <--
JP 3296490	B2	20020702	JP 1994-501089	19930603 <--
CN 1082318	A	19940223	CN 1993-108296	19930604 <--
IL 105909	A1	19970415	IL 1993-105909	19930604 <--

PRIORITY APPLN. INFO.: EP 1992-109525 A 19920605
WO 1993-EP1406 A 19930603

OTHER SOURCE(S): MARPAT 120:270104
GI



I

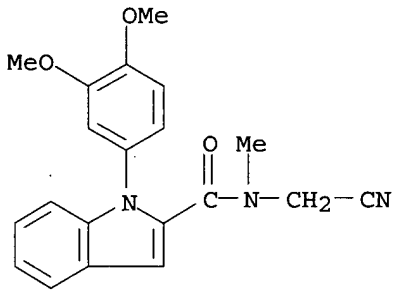
AB Title compds. I (R = substituted Ph; R3, R4 = H , halo, (substituted) alkyl, -alkoxy, -cycloalkyl, -Ph, -PhO; R5, R6 = H, (substituted) alkyl, -alkoxy, -cycloalkyl, =Ph, -heterocyclyl; R5R6N = heterocyclyl; R7 = H, alkyl) useful as agrochem. fungicidal compns., are prepared 4-Bromoveratrole, Et indole-2-carboxylate, K2CO3, Cu(I)bromide, pyridine and nitrobenzene were stirred at 140° for 14 h, to give after cooling to room temperature Et 1-(3,4-dimethoxyphenyl)indole-2-carboxylate which was converted to the free acid and this stirred in CCl4 and N,N'-carbonyldiimidazole was refluxed, morpholine was added and refluxed to give I [R = 3,4-(MeO)2C6H3, R3 = R4 = R7 = H, R5R6N = morpholin-4-yl].

A similar prepared I [R = 3,4-(MeO)2C6H3, R3 = 5-Me3C, R4 = R7 = H, R5R6N = morpholin-4-yl] tested against Phytophthora infestans agar culture showed a min. inhibitory concentration of 0.2 μg/mL vs. 0.78 μg/mL for control. I were also active against vine downy mildew and tomato late blight.

IT **154536-90-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as agrochem. fungicide)

RN 154536-90-0 HCAPLUS

CN 1H-Indole-2-carboxamide, N-(cyanomethyl)-1-(3,4-dimethoxyphenyl)-N-methyl- (9CI) (CA INDEX NAME)



L12 ANSWER 22 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:77256 HCAPLUS

DOCUMENT NUMBER: 120:77256

TITLE: Novel synthesis of 2-acyl-1,2,3,6,7,11b-hexahydropyrazino[2,1-a]isoquinolin-4-ones based on acylglycine 2-phenylethylamide N-cyanomethyl derivatives

AUTHOR(S): Shekhter, O. V.; Kuklenkova, O. B.; Sergovskaya, N. L.; Tsizin, Yu. S.

CORPORATE SOURCE: Inst. Med. Parazitol. Trop. Med. im. Martsinovskogo, Moscow, 119435, Russia

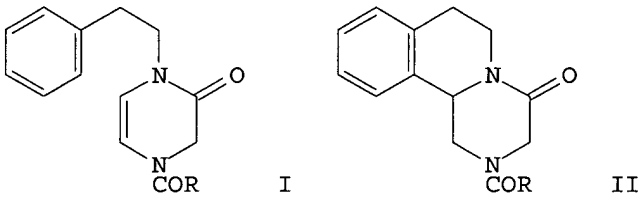
SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (**1993**), (2), 197-201
CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 120:77256

GI

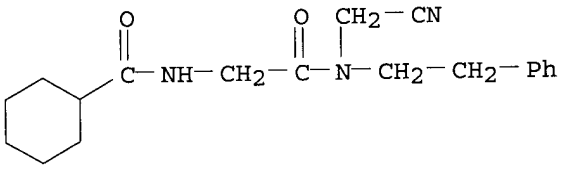


AB Hippuric acid and (cyclohexylcarbonyl)glycine condensed with PhCH2CH2NHCH2CN in the presence of DCC to give 77-78% PhCH2CH2N(CH2CN)COCH2NHCOR (R = Ph, cyclohexyl, resp.), which underwent reductive cyclization with 50% HCHO and Raney Ni to give 53-63% dehydropiperazinones I (same R). Intramol. cycloaddn. reaction of I in

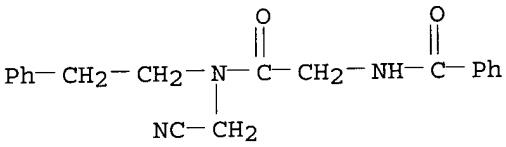
the presence of H2SO4 gave 70-83% title compds. II (same R). Condensing glycine with aqueous HCHO and KCN and then treating with BzCl gave 67% NCCH2NBzCH2CO2H, which condensed with PhCH2CH2NH2 as above to give 62% PhCH2CH2NHCOCH2NBzCH2CN (III). Reductive cyclization of III as above yielded 45% I (R = Ph) and 23% hydrated analog, and the mixture was treated with H2SO4 to give 68% II (R = Ph).

IT **152189-66-7P 152189-68-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive intramol. cyclization of)

RN 152189-66-7 HCAPLUS
CN Cyclohexanecarboxamide, N-[2-[(cyanomethyl)(2-phenylethyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



RN 152189-68-9 HCAPLUS
CN Benzamide, N-[2-[(cyanomethyl)(2-phenylethyl)amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)



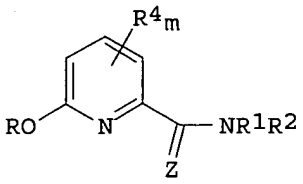
L12 ANSWER 23 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:	1993:539127 HCAPLUS
DOCUMENT NUMBER:	119:139127
TITLE:	Preparation of 2-(pyridyloxy)-6-pyridinecarboxamides as herbicides
INVENTOR(S):	Bissinger, Hans Joachim; Kleemann, Axel; Searle, Richard J. G.
PATENT ASSIGNEE(S):	Shell Internationale Research Maatschappij B. V., Neth.
SOURCE:	Can. Pat. Appl., 78 pp. CODEN: CPXXEB
DOCUMENT TYPE:	Patent
LANGUAGE:	English
FAMILY ACC. NUM. COUNT:	1

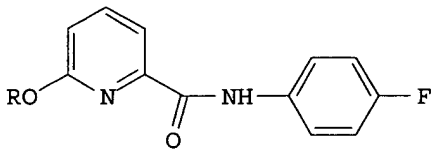
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
CA 2078026	AA	19930314	CA 1992-2078026		19920911 <--
PRIORITY APPLN. INFO.:			DE 1991-9111554	U	19910913

OTHER SOURCE(S): MARPAT 119:139127
GI



I



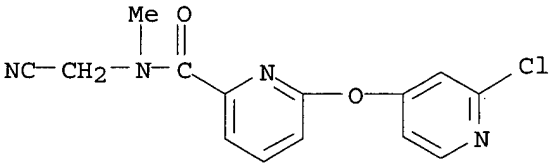
II

AB Title compds. [I; R = (substituted)pyridyl; R1, R2 = H, (cyclo)alkyl, alkenyl, aryl, OH, alkoxy, etc.; R4 = halo, (halo)alkyl; Z = O, S; m = 0-3] were prepared Thus, 6-chloropicolinic acid was condensed with 4-FC6H4NH2 and the product condensed with 2-chloro-4-pyridinol to give title compound II (R = 2-chloro-4-pyridyl). II (R = 3-pyridyl) gave 70-80% and 80-90% control of Echinochloa crus-galli and Sinapsis alba, resp., with 0-10% damage to, e.g., corn.

IT **149527-89-9P 149528-86-9P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

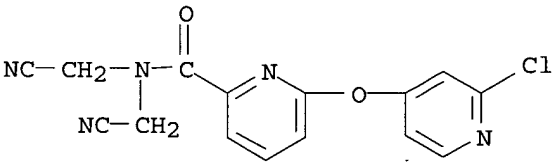
RN 149527-89-9 HCAPLUS

CN 2-Pyridinecarboxamide, 6-[(2-chloro-4-pyridinyl)oxy]-N-(cyanomethyl)-N-methyl- (9CI) (CA INDEX NAME)



RN 149528-86-9 HCAPLUS

CN 2-Pyridinecarboxamide, 6-[(2-chloro-4-pyridinyl)oxy]-N,N-bis(cyanomethyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 24 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:263757 HCAPLUS

DOCUMENT NUMBER: 118:263757

TITLE: Silver halide photographic material

INVENTOR(S): Kawashima, Yasuhiko; Yamauchi, Reiko; Kojima, Tamotsu; Kagawa, Nobuaki

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 27 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

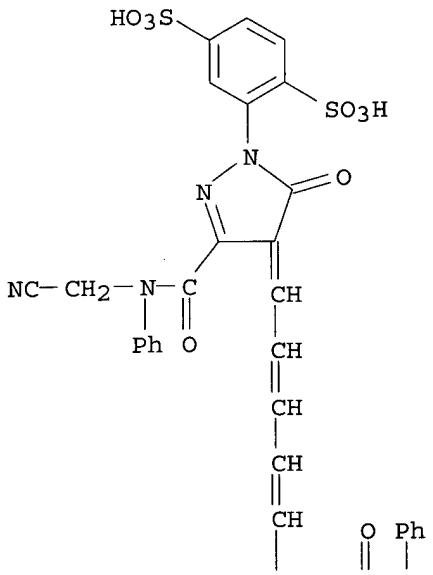
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

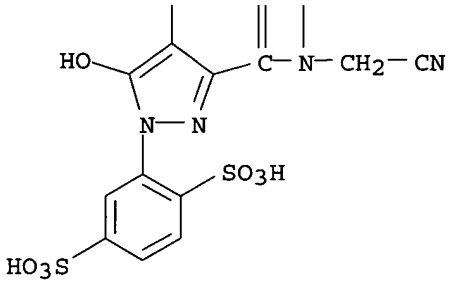
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04229856	A2	19920819	JP 1990-415096	19901227 <--
PRIORITY APPLN. INFO.:			JP 1990-415096	19901227

OTHER SOURCE(S): MARPAT 118:263757
GI For diagram(s), see printed CA Issue.
AB A Ag halide photog. material contains a compound I [R1-R2 = H, alkyl, aryl, alkenyl; R3, R5 = alkyl, alkenyl; R4, R6 = aryl; L1-L6 = methine chain; n1, n2 = 0, 1, 2. The compound has a good spectroscopic absorption property, is photog. inactive, and does not contaminate developer solution
IT **147841-57-4**
RL: TEM (Technical or engineered material use); USES (Uses)
(silver halide photog. materials containing)
RN 147841-57-4 HCAPLUS
CN 1,4-Benzenedisulfonic acid, 2-[3-[[(cyanomethyl)phenylamino]carbonyl]-4-[5-[3-[[(cyanomethyl)phenylamino]carbonyl]-1-(2,5-disulfophenyl)-1,5-dihydro-5-oxo-4H-pyrazol-4-ylidene]-1,3-pentadienyl]-5-hydroxy-1H-pyrazol-1-yl]-, tetrapotassium salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



●4 K

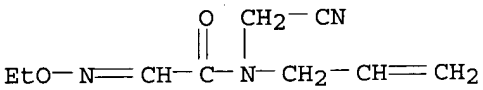
L12 ANSWER 25 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:71110 HCAPLUS
DOCUMENT NUMBER: 110:71110
TITLE: Preparation of iminoacetic acid derivatives as fungicides.
INVENTOR(S): Kojima, Shigeru; Matsuhashi, Taisuke; Hayakawa, Koichi; Hashimoto, Akira; Shimoda, Susumu; Haramoto, Masanori; Nakada, Akira
PATENT ASSIGNEE(S): Nippon Soda Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63162673	A2	19880706	JP 1986-315017	19861225 <--
JP 2556317	B2	19961120		
PRIORITY APPLN. INFO.:			JP 1986-315017	19861225

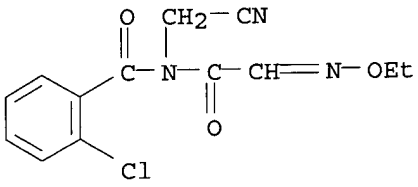
OTHER SOURCE(S): MARPAT 110:71110
AB ACOCH:NXR [I; R = (substituted)alkyl, cycloalkyl, halo- or NO2-substituted Ph, etc.; X = O, S; A = R1R2N, R3Y; R1,R2 = H, OH, cyano, acyl, aroyl,(substituted)alkyl, cycloalkyl, (substituted)Ph, (substituted)pyridyl, etc.; R3 = H, cation, (substituted) alkyl, (substituted) Ph, amino, 5-membered heterocyclyl, etc.; Y = O, S], useful as agrochem. fungicides, are prepared To a stirred mixture of 15.8 g N-(2-chloroethoxy)phthalimide and EtOH at .apprx.0° was added dropwise H2NNH2.H2O. The resulting solution was stirred 2.5 h at room temperature, followed by filtration and addition of 40% aqueous glyoxylic acid at -4° to give 6.6 g I (R = ClCH2CH2, X = O, A = OH) (II). A wettable powder was formulated by grinding a mixture of II 40, Kieselguhr 53, higher alc. sulfate ester 4, and alkylnaphthalenesulfonic acid 3 weight parts. II, at 200 ppm, showed complete control of Pellicularia filamentosa and Pseudopernospora cubensis on cucumbers and Phytophthora infestans on tomatoes, with no damage on the cucumbers and tomatoes.
IT **118568-19-7P 118568-67-5P 118568-73-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as agrochem. fungicide)

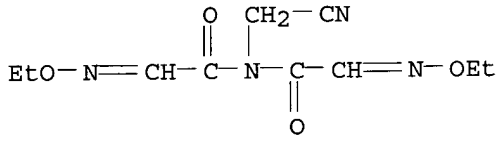
RN 118568-19-7 HCAPLUS
CN Acetamide, N-(cyanomethyl)-2-(ethoxyimino)-N-2-propenyl- (9CI) (CA INDEX NAME)



RN 118568-67-5 HCAPLUS
CN Benzamide, 2-chloro-N-(cyanomethyl)-N-[(ethoxyimino)acetyl]- (9CI) (CA INDEX NAME)



RN 118568-73-3 HCAPLUS
CN Acetamide, N-(cyanomethyl)-2-(ethoxyimino)-N-[(ethoxyimino)acetyl]- (9CI) (CA INDEX NAME)



L12 ANSWER 26 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:204232 HCAPLUS
DOCUMENT NUMBER: 108:204232
TITLE: Preparation of N-(2-cyano-2-oximinoacetyl)aminonitriles as fungicides
INVENTOR(S): Lunkenheimer, Winfried; Berg, Dieter; Brandes, Wilhelm
PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 29 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3625460	A1	19880204	DE 1986-3625460	19860728 <--
EP 256326	A1	19880224	EP 1987-110468	19870720 <--
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, NL, SE				
AU 8776114	A1	19880204	AU 1987-76114	19870723 <--
JP 63035554	A2	19880216	JP 1987-183779	19870724 <--

DD 263439	A5	19890104	DD 1987-305324		19870724 <--
DK 8703903	A	19880129	DK 1987-3903		19870727 <--
BR 8703868	A	19880329	BR 1987-3868		19870727 <--
ZA 8705491	A	19880427	ZA 1987-5491		19870727 <--
HU 45007	A2	19880530	HU 1987-3462		19870728 <--
PRIORITY APPLN. INFO.:			DE 1986-3625460	A	19860728

OTHER SOURCE(S): CASREACT 108:204232; MARPAT 108:204232

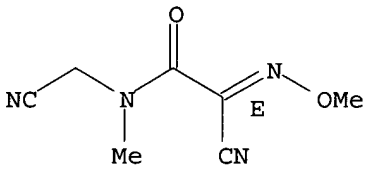
AB R1ON:C(CN)CONR2ACN [I; R1 = (substituted) cycloalkyl, CHR3X; X = H, alkyl, alkenyl, cyano, hydroxy-, alkoxy-, or aminocarbonyl etc.; R3 = H, alkyl; R2 = H, alkyl; R2NA = heterocycle; A = (substituted) alkylene] are prepared as agrochem. fungicides. A DMF solution of 0.05 mol methylaminoacetonitrile hydrochloride and 0.1 mol Et3N at 0° was treated dropwise with 0.05 mol (E)-2-cyano-2-methoximinoacetyl chloride and stirred 1 h at 0° and 18 h at room temperature to give 5.7 g I (R1 = R2 = Me, A = CH2) (II). In tests against Phytophthora infestans on tomato plants, II proved superior to [SC(S)NHCH2CH2NHC(S)SZn]x (x undefined).

IT **114314-07-7P 114314-10-2P 114314-15-7P**
114332-42-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as fungicide)

RN 114314-07-7 HCAPLUS

CN Acetamide, 2-cyano-N-(cyanomethyl)-2-(methoxyimino)-N-methyl-, (E)- (9CI) (CA INDEX NAME)

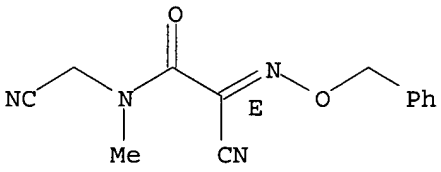
Double bond geometry as shown.



RN 114314-10-2 HCAPLUS

CN Acetamide, 2-cyano-N-(cyanomethyl)-N-methyl-2-[(phenylmethoxy)imino]-, (E)- (9CI) (CA INDEX NAME)

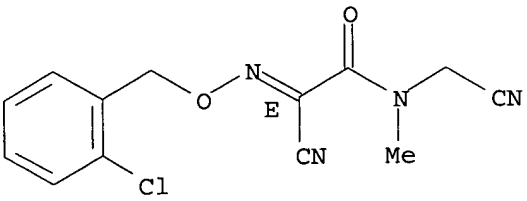
Double bond geometry as shown.



RN 114314-15-7 HCAPLUS

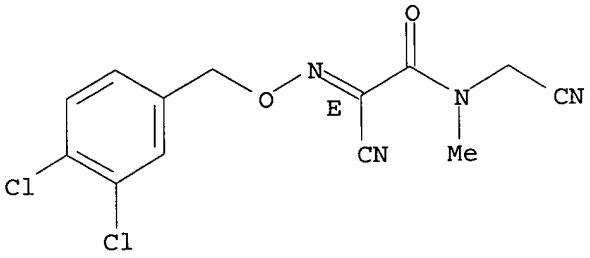
CN Acetamide, 2-[[(2-chlorophenyl)methoxy]imino]-2-cyano-N-(cyanomethyl)-N-methyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 114332-42-2 HCAPLUS
CN Acetamide, 2-cyano-N-(cyanomethyl)-2-[[(3,4-dichlorophenyl)methoxy]imino]-N-methyl-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L12 ANSWER 27 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:213424 HCAPLUS
DOCUMENT NUMBER: 106:213424
TITLE: Fungicidal cyano oximes for plants
INVENTOR(S): Kay, Ian Trevor; Crowley, Patrick Jelf; Bartholomew, David; Shephard, Margaret Clair; Heaney, Stephen Paul
PATENT ASSIGNEE(S): Imperial Chemical Industries PLC, UK
SOURCE: Brit. UK Pat. Appl., 39 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2173791	A1	19861022	GB 1986-6647	19860318 <--
GB 2173791	B2	19890705		
EP 201999	A1	19861120	EP 1986-301986	19860318 <--
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
ZA 8602242	A	19861126	ZA 1986-2242	19860325 <--
AU 8655267	A1	19861023	AU 1986-55267	19860326 <--
BR 8601644	A	19861216	BR 1986-1644	19860411 <--
HU 41206	A2	19870428	HU 1986-1546	19860414 <--
DK 8601736	A	19861017	DK 1986-1736	19860416 <--
JP 61243057	A2	19861029	JP 1986-86224	19860416 <--
CN 86102450	A	19870218	CN 1986-102450	19860416 <--
ES 554025	A1	19870601	ES 1986-554025	19860416 <--

PRIORITY APPLN. INFO.:

GB 1985-9733	A	19850416
GB 1985-21390	A	19850828
GB 1985-31283	A	19851219
GB 1986-6647	A	19860318

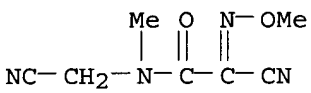
OTHER SOURCE(S): CASREACT 106:213424

AB The title plant fungicides R1R2NCOC(CN):NOR (I; R = H, alkyl, cycloalkyl, cycloalkylalkyl, (un)substituted alkenyl, -alkynyl, -PhCH2, metal ion; R1 = (un)substituted alkenyl, -alkynyl, -cyanoalkyl, -heterocyclyl, -allenylmethyl, etc.; R2 = H, (un)substituted cyanoalkyl, -alkenyl, -alkynyl, -allenylmethyl) useful as plant fungicides, were prepared Thus, EtO2CC(CN):NOH in MeCN was alkylated with MeI to give EtO2CC(CN):NOMe which was reacted with HC.tplbond.CCH2NH2.HCl and Et3N to give I (R = Me, R1 = HC.tplbond.CCH2, R2 = H) (II). II in a suspension formulation applied to potted plants 1 or 2 days before the plant was inoculated with the pathogen, and assessed 4-14 days later showed complete control of Puccinia recondita (wheat) and Plasmopara viticola (vines). Various formulations containing I are given.

IT **107792-09-6P 107792-17-6P 107792-18-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as plant fungicide)

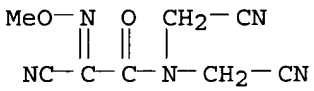
RN 107792-09-6 HCAPLUS

CN Acetamide, 2-cyano-N-(cyanomethyl)-2-(methoxyimino)-N-methyl- (9CI) (CA INDEX NAME)



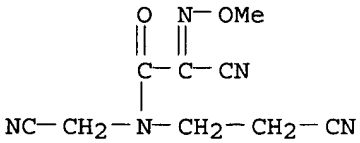
RN 107792-17-6 HCAPLUS

CN Acetamide, 2-cyano-N,N-bis(cyanomethyl)-2-(methoxyimino)- (9CI) (CA INDEX NAME)



RN 107792-18-7 HCAPLUS

CN Acetamide, 2-cyano-N-(2-cyanoethyl)-N-(cyanomethyl)-2-(methoxyimino)- (9CI) (CA INDEX NAME)



L12 ANSWER 28 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:406801 HCAPLUS

DOCUMENT NUMBER: 105:6801

TITLE: Rapid and convenient syntheses of polyoxin peptides containing N-methylated peptide bonds

AUTHOR(S): Boehm, Jeffrey C.; Kingsbury, William D.

CORPORATE SOURCE: Dep. Med. Chem., Smith Kline and French Lab., Swedeland, PA, 19479, USA

SOURCE: Journal of Organic Chemistry (**1986**), 51(12), 2307-14
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 105:6801
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

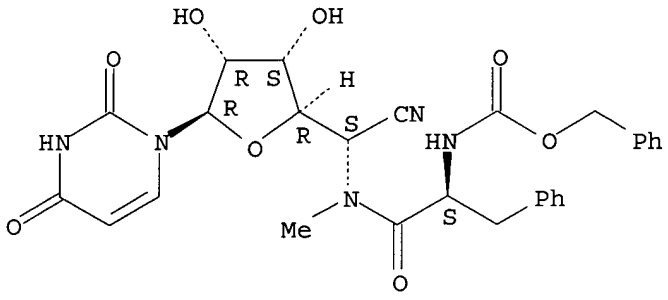
AB N-Methylated polyoxin dipeptides L, D-I and L, L-I (R = OH) and tripeptide L, L, L-I (R = NHCHMeCO2H) (II) were prepared using the Ugi 4-component condensation reaction. Thus, the Ugi reaction of uridine aldehyde III with MeNH2, Z-Phe-OH (Z = PhCH2O2C), and DL-CNCHMeCO2CH2Ph gave a diastereoisomeric mixture of tripeptide derivative IV, which was cleaved by refluxing 50% HOAc to give uridine derivative V. The diastereoisomer of V were separated by HPLC and the L, L, L-isomer of V was deblocked by catalytic hydrogenation using HCO2H in MeOH over Pd to give II. Alternatively, entry into the dipeptide system was achieved by a short synthesis based upon the Strecker reaction. Polyoxin amides L, D- and L, L-VI (R1 = CONH2) and polyoxin nitrile L, D-VI (R1 = CN) were also prepared

IT **100683-01-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and catalytic transfer hydrogenation of)

RN 100683-01-0 HCAPLUS

CN α-L-Talofuranurononitrile, 1,5-dideoxy-1-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-5-[methyl[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

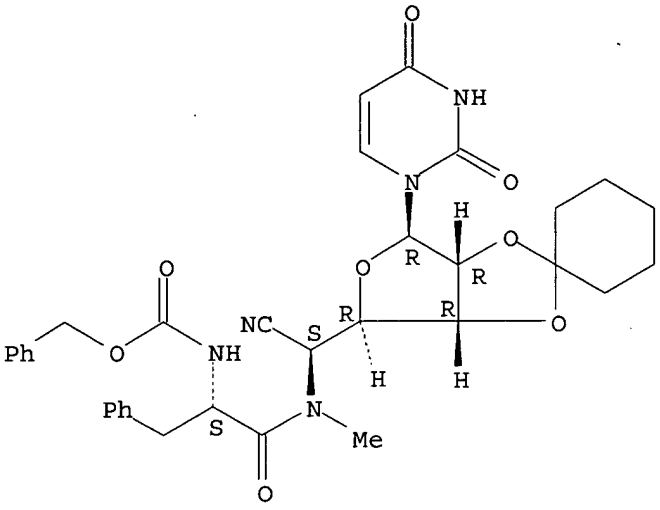


IT **100682-90-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 100682-90-4 HCAPLUS

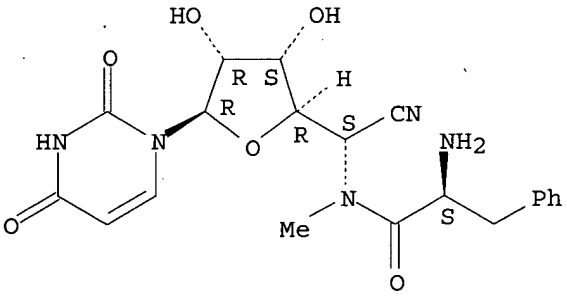
CN α-L-Talofuranurononitrile, 2,3-O-cyclohexylidene-1,5-dideoxy-1-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-5-[methyl[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

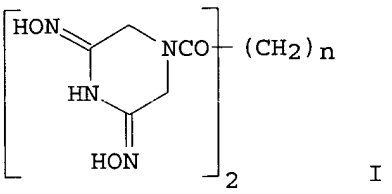


IT **100682-95-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 100682-95-9 HCAPLUS
CN α-L-Talofuranurononitrile, 5-[(2-amino-1-oxo-3-phenylpropyl)methylamino]-1,5-dideoxy-1-(3,4-dihydro-2,4-dioxo-1(2H)-pyrimidinyl)-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L12 ANSWER 29 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:78831 HCAPLUS
DOCUMENT NUMBER: 102:78831
TITLE: Some derivatives of bisdioxopiperazines and their biological activity
AUTHOR(S): Cekuoliene, L.; Simkeviciene, V.; Kersulis, A.; Zhavrid, S. V.; Shashikhina, M. N.
CORPORATE SOURCE: USSR
SOURCE: Tsitol., Immunol. Biokhim. Izuch. Leikoznoi Kletki (**1983**), 171-7. Editor(s): Sadauskas, P. B. Akad. Nauk Litov. SSR, Inst. Biokhim.: Vilnius, USSR. CODEN: 52NOAG
DOCUMENT TYPE: Conference
LANGUAGE: Russian
GI



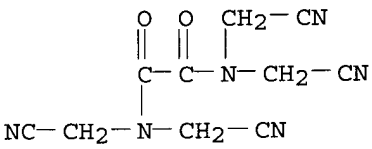
I

AB Piperazinediones I (n = 0 or 2) were prepared by condensing [(NCCH2)2NCO]2(CH2)n with NH2OH.HCl in dioxane-MeOH-H2O in the presence Na2CO3. The I showed weak antitumor activity (and low toxicity) in mice.

IT **73502-40-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with heterooxylamine)

RN 73502-40-6 HCAPLUS

CN Ethanediamide, tetrakis(cyanomethyl)- (9CI) (CA INDEX NAME)



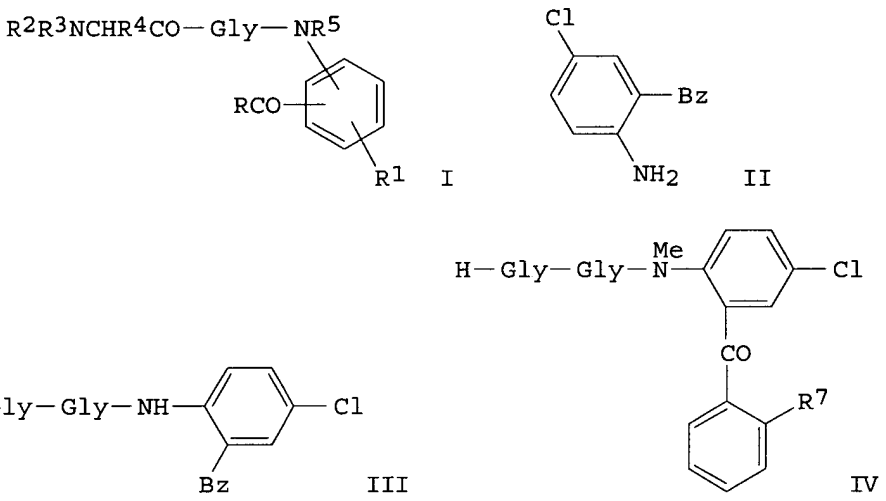
L12 ANSWER 30 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:35726 HCAPLUS
DOCUMENT NUMBER: 96:35726
TITLE: Dipeptide derivatives
INVENTOR(S): Hirai, Kentaro; Ishiba, Teruyuki; Sasakura, Kazuyuki; Sugimoto, Hirohiko
PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
SOURCE: Can., 41 pp.
CODEN: CAXXA4
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 1091652	A2	19801216	CA 1979-339232	19791106 <--
JP 51026853	A2	19760305	JP 1974-90565	19740806 <--
JP 60004199	B4	19850201		
ZA 7504877	A	19760728	ZA 1975-4877	19750729 <--
CA 1181065	A1	19850115	CA 1975-232782	19750731 <--
BE 832190	A1	19751201	BE 1975-158997	19750806 <--
US 4076702	A	19780228	US 1976-716265	19760820 <--
US 4076703	A	19780228	US 1976-716266	19760820 <--
US 4076704	A	19780228	US 1976-716267	19760820 <--
US 4076705	A	19780228	US 1976-716268	19760820 <--
US 4240957	A	19801223	US 1977-775646	19770307 <--
US 4154727	A	19790515	US 1978-867605	19780106 <--
CH 627438	A	19820115	CH 1979-4617	19790517 <--
CH 627439	A	19820115	CH 1979-4618	19790517 <--

CH 627440	A	19820115	CH 1979-8270		19790912 <--
PRIORITY APPLN. INFO.:			JP 1974-905566	A	19740806
			JP 1974-90565	A	19740806
			CA 1975-232782	A3	19750731
			JP 1966-9055	A	19740806
			JP 1974-90566	A	19740806
			US 1975-601134	A3	19750801
			CH 1975-10202	A	19750805
			US 1977-775646	A3	19770307

GI

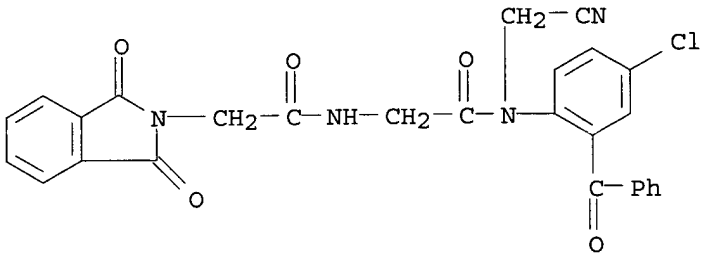


AB Dipeptide anilides I (R = benzene or pyridine ring optionally substituted with halogen; R1 = halo; R2 = H, C1-6 alkyl, C7-14 aralkyl, glycyl, glycylglycyl; R3 = H, C1-6 alkyl, NH2-protective group; R2R3N = phthalimido, piperidino, 4-hydroxy-4-(p-halophenyl)piperidino, morpholino, or piperazino substituted by C1-6 alkyl or Ph; R4 = H, Me, CHMe2, CH2CHMe2, CH2Ph, Ph; R5 = H, C1-6 alkyl, C2-7 cyanoalkyl, C3-10 dialkylaminoalkyl) were prepared as anxiolytics, sedatives, anticonvulsives, hypnotics, and muscle relaxants. Thus, Ph3C-Gly-Gly-OH was treated with SOCl2 in hexamethylphosphoric triamide to give the acid chloride, which was amidated with benzophenone II to give dipeptide anilide III (R6 = Ph3C), which was detritylated by 50% HOAc to give III (R6 = H). Many other I derivs., including anilides IV (R7 = H, Cl), were also prepared Anti-pentylenetetrazole activity, taming activity, and rotarod performance activity of IV in mice were determined

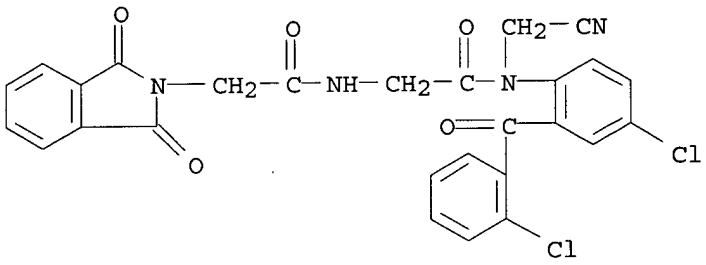
IT **59180-22-2P 59180-23-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrazine anal. of)

RN 59180-22-2 HCAPLUS

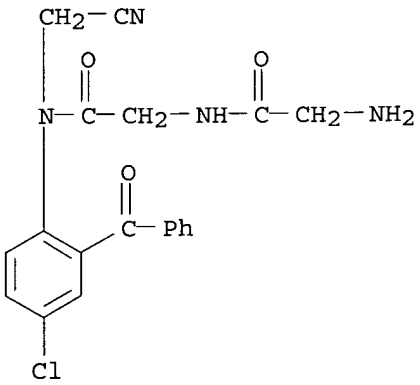
CN 2H-Isoindole-2-acetamide, N-[2-[(2-benzoyl-4-chlorophenyl)(cyanomethyl)amino]-2-oxoethyl]-1,3-dihydro-1,3-dioxo- (9CI) (CA INDEX NAME)



RN 59180-23-3 HCAPLUS
CN 2H-Isoindole-2-acetamide, N-[2-[[4-chloro-2-(2-chlorobenzoyl)phenyl](cyanomethyl)amino]-2-oxoethyl]-1,3-dihydro-1,3-dioxo- (9CI) (CA INDEX NAME)



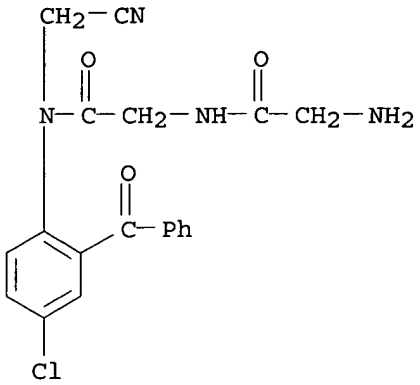
IT **59180-24-4P 59180-25-5P 59180-26-6P 59180-27-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59180-24-4 HCAPLUS
CN Glycinamide, glycyl-N-(2-benzoyl-4-chlorophenyl)-N-(cyanomethyl)- (9CI) (CA INDEX NAME)



RN 59180-25-5 HCAPLUS
CN Glycinamide, glycyl-N-(2-benzoyl-4-chlorophenyl)-N-(cyanomethyl)-, 2-hydroxy-1,2,3-propanetricarboxylate (2:1) (9CI) (CA INDEX NAME)

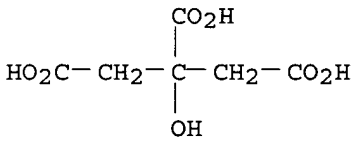
CM 1

CRN 59180-24-4
CMF C19 H17 Cl N4 O3

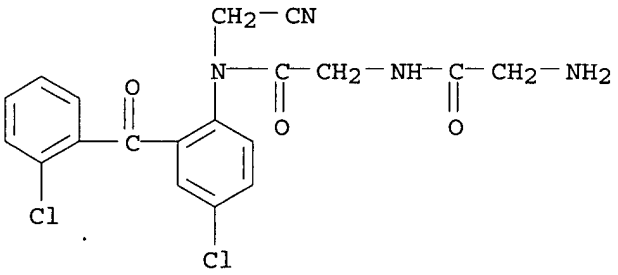


CM 2

CRN 77-92-9
CMF C6 H8 O7



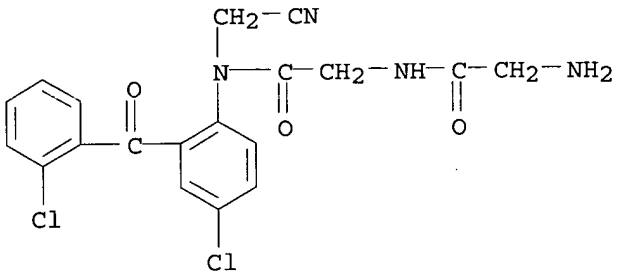
RN 59180-26-6 HCAPLUS
CN Glycinamide, glycyl-N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-(cyanomethyl)-(9CI) (CA INDEX NAME)



RN 59180-27-7 HCAPLUS
CN Glycinamide, glycyl-N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-(cyanomethyl)-, 2-hydroxy-1,2,3-propanetricarboxylate (2:1) (9CI) (CA INDEX NAME)

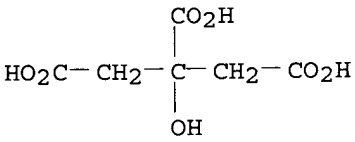
CM 1

CRN 59180-26-6
CMF C19 H16 Cl2 N4 O3



CM 2

CRN 77-92-9
CMF C6 H8 O7

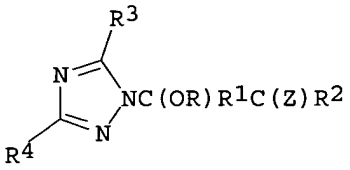


L12 ANSWER 31 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:15736 HCAPLUS
DOCUMENT NUMBER: 94:15736
TITLE: Fungicidal 1,2,4-triazol-1-yl compounds
INVENTOR(S): Stubenrauch, Gerd; Ammermann, Eberhard; Pommer, Ernst Heinrich
PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 52 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2846127	A1	19800430	DE 1978-2846127	19781023 <--
EP 10298	A1	19800430	EP 1979-104020	19791018 <--
EP 10298	B1	19811209		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
SU 1055313	A3	19831115	SU 1979-2830605	19791018 <--
DD 146686	C	19810225	DD 1979-216344	19791019 <--
IL 58506	A1	19840229	IL 1979-58506	19791019 <--
PL 118865	B2	19811130	PL 1979-219083	19791020 <--
DK 7904443	A	19800424	DK 1979-4443	19791022 <--
ZA 7905629	A	19801126	ZA 1979-5629	19791022 <--
CA 1132580	A1	19820928	CA 1979-338144	19791022 <--
CS 221276	P	19830429	CS 1979-7154	19791022 <--
HU 25796	O	19830829	HU 1979-BA3871	19791022 <--
HU 183082	B	19840428		

PRIORITY APPLN. INFO.: DE 1978-2846127 A 19781023

GI



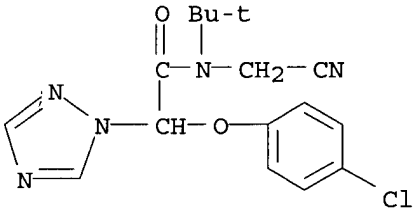
I

AB The triazole derivs. I [R = (substituted) aryl or heteroaryl; R1 = H, (substituted) (cyclo) aliphatic group, aryl, aralkyl, or heteroaryl; R2 = OR5, SR5 (R5 = aliphatic, aryl, heteraryl, etc.) or (substituted) NH2; Z = O, S; R3, R4 = H, halogen, NO2, alkyl] were prepared for use as fungicides (test data tabulated). Thus, 1,2,4-triazole reacted with 4-PhC6H4OCHBrCO2Me in THF to give 81% I (R = 4-PhC6H4, R1 = R3 = R4 = H, CZR2 = CO2Me).

IT **75470-14-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 75470-14-3 HCAPLUS

CN 1H-1,2,4-Triazole-1-acetamide, α-(4-chlorophenoxy)-N-(cyanomethyl)-N-(1,1-dimethylethyl)- (9CI) (CA INDEX NAME)



L12 ANSWER 32 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:180653 HCAPLUS

DOCUMENT NUMBER: 92:180653

TITLE: Synthesis and study of the antiinflammatory activity of derivatives of dicarboxylic acids

AUTHOR(S): Astrauskas, V.; Cekuoliene, L.; Svedaite, I.

CORPORATE SOURCE: USSR

SOURCE: Metab. Ego Regul. Biol. Akt. Veshchestvami (**1979**), 82-8. Editor(s): Kanopkaite, S. I. Akad. Nauk Lit. SSR, Inst. Biokhim.: Vilnius, USSR. CODEN: 42DDAO

DOCUMENT TYPE: Conference

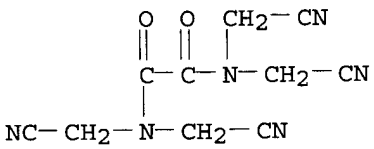
LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 92:180653

AB Treatment of [(MeO2CCH2)2NCOX]2 (X = bond, CH2) with H2NCH2CH2OH gave [(HOCH2CH2NHCOCH2)2NCOX]2 (I) in 50 and 51% yield, resp. [(NCCH2)2NCOX] (II; X = band, CH2) were prepared in 77 and 70% yield, resp., by reaction of HN(CH2CN)2 with (ClCOX)2. The antiinflammatory activity of I was determined earlier (Astrauskas et.al., 1977). II have an insignificant amount of antiinflammatory activity.

IT **73502-40-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

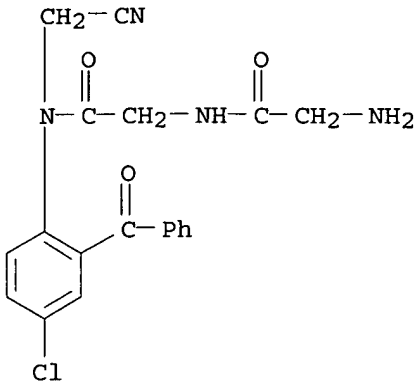
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and antiinflammatory activity of)
RN 73502-40-6 HCAPLUS
CN Ethanediamide, tetrakis(cyanomethyl)- (9CI) (CA INDEX NAME)



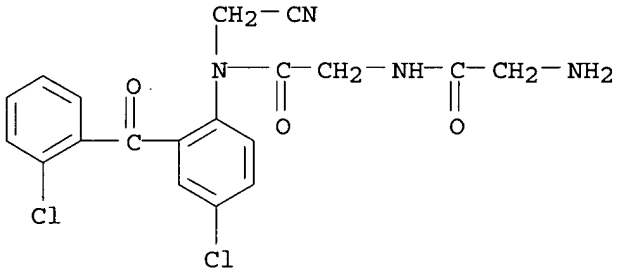
L12 ANSWER 33 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1978:62614 HCAPLUS
DOCUMENT NUMBER: 88:62614
TITLE: Dipeptide derivatives
INVENTOR(S): Hirai, Kentaro; Ishiha, Teruyuki; Sasakura, Kazuyuki; Sugimoto, Hirohiko
PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52083722	A2	19770712	JP 1976-313	19760101 <--
JP 59042668	B4	19841016		
PRIORITY APPLN. INFO.:			JP 1976-313 A	19760101

GI For diagram(s), see printed CA Issue.
AB Forty-two title derivs. I [R = H, alkyl, alkenyl, etc.; R1, R2 = H alkyl, aralkyl, etc.; R3 = H, alkyl, NH2-protecting groups; R1R2 may form an alkylene group; NR2R3 may be phthalimido, piperidino, other heterocyclics; ring A = un- or halo-substituted benzene or pyridine; ring B = (un)substituted benzene or substituted thiophene] and their acid salts were prepared, e.g., by reaction of II with R2NR3CHR1CONHCH2CO2H. Thus, 5 g tritylglycylglycine in (Me2N)3PO was stirred with 1.6 g SOCl2 20 min at -5°, 3.08 g 5,2-Cl(H2N)C6H3COPh was added, and the mixture was kept overnight at room temperature to give 1.7 g 2-benzoyl-4-chloro-N-tritylglycylglycinanilide (III). Heating 1.7 g III in 50% AcOH 20 min on a water bath gave 0.8 g 2-benzoyl-4-chloroglycylglycinanilide (IV). I are useful as tranquilizers, anticonvulsants, hypnotics, and muscle-relaxants; the data on IV and 2 other I were given in mice in comparison with chlordiazepoxide and diazepam. LD50 of IV was 1309 mg/kg in mice.
IT **59180-24-4P 59180-26-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59180-24-4 HCAPLUS
CN Glycinamide, glycyl-N-(2-benzoyl-4-chlorophenyl)-N-(cyanomethyl)- (9CI) (CA INDEX NAME)



RN 59180-26-6 HCAPLUS
CN Glycinamide, glycyl-N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-(cyanomethyl)-
(9CI) (CA INDEX NAME)



L12 ANSWER 34 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:584551 HCAPLUS
DOCUMENT NUMBER: 87:184551
TITLE: Quinoxaline di-N-oxide derivatives
INVENTOR(S): Schmid, Wolfgang; Basler, Walter; Burckhardt, Urs
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.
SOURCE: Ger. Offen., 20 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2701707	A1	19770721	DE 1977-2701707	19770117 <--
DE 2701707	C2	19860522		
GB 1569034	A	19800611	GB 1977-2356	19760120 <--
CH 627174	A	19811231	CH 1976-634	19760120 <--
SU 890961	A3	19811215	SU 1977-2437355	19770110 <--
CA 1108143	A1	19810901	CA 1977-269894	19770118 <--
BE 850510	A1	19770719	BE 1977-174182	19770119 <--
DK 7700202	A	19770721	DK 1977-202	19770119 <--
DK 141509	B	19800408		
DK 141509	C	19800929		

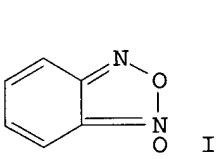
SE 7700529	A	19770721	SE 1977-529	19770119	<--
SE 427928	B	19830524			
SE 427928	C	19830901			
FR 2338935	A1	19770819	FR 1977-1398	19770119	<--
FR 2338935	B1	19790323			
BR 7700355	A	19770920	BR 1977-355	19770119	<--
AU 7721443	A1	19780727	AU 1977-21443	19770119	<--
AU 515192	B2	19810319			
IL 51292	A1	19810629	IL 1977-51292	19770119	<--
NL 7700581	A	19770722	NL 1977-581	19770120	<--
JP 52089683	A2	19770727	JP 1977-5395	19770120	<--
JP 61035985	B4	19860815			
HU 175068	P	19800528	HU 1977-CI1714	19770120	<--
DK 7803943	A	19780906	DK 1978-3943	19780906	<--
DK 146388	B	19830926			
DK 146388	C	19840305			

PRIORITY APPLN. INFO.:

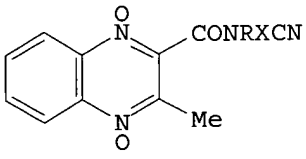
CH 1976-634	A	19760120
CH 1976-14920	A	19761126
CH 1976-643	A	19761120
DK 1977-202	A	19770119

OTHER SOURCE(S): CASREACT 87:184551

GI



I



II

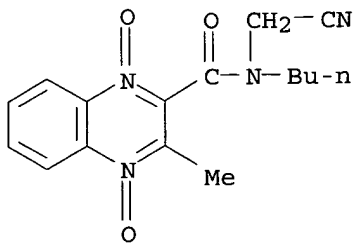
AB Cyclization of benzofuroxan (I) with AcCH2CONRXCN gave 15 quinoxaline dioxides II (R = H, Me, CH2CH2CN, Bu, dodecyl, CH2CH:CH2, hexyl; X = CH2, CMe2, CH2CH2, CH2CHMe, CHMe, (CH2)3, (CH2)4, CHEt, CHMe). Thus, 23.8 gms AcCH2CONHCH2CH2CN was cyclized with 19.2 gms I to give II (R = H, X = CH2CH2), useful as an animal growth promoter. Extensive data was given for the effectiveness of II (R = H, X = CH2, CMe2) as bactericides against 6-bacteria including Staphlococcus aureus, Escherichia coli and Pseudomonas aeruginosa.

IT **64557-88-6P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 64557-88-6 HCAPLUS

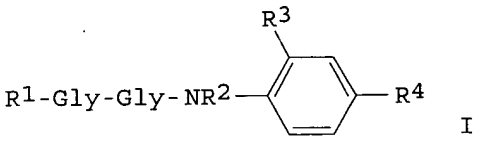
CN 2-Quinoxalinecarboxamide, N-butyl-N-(cyanomethyl)-3-methyl-, 1,4-dioxide (9CI) (CA INDEX NAME)



L12 ANSWER 35 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:180642 HCAPLUS
DOCUMENT NUMBER: 84:180642
TITLE: Dipeptide derivatives
INVENTOR(S): Hirai, Kentaro; Ishiba, Teruyuki; Sasakura, Kazuyuki; Sugimoto, Hirohiko
PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
SOURCE: Ger. Offen., 40 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2535171	A1	19760219	DE 1975-2535171	19750806 <--
DE 2535171	B2	19790523		
DE 2535171	C3	19800124		
JP 51026853	A2	19760305	JP 1974-90565	19740806 <--
JP 60004199	B4	19850201		
JP 51026854	A2	19760305	JP 1974-90566	19740806 <--
JP 60005599	B4	19850212		
ZA 7504877	A	19760728	ZA 1975-4877	19750729 <--
NL 7509258	A	19760210	NL 1975-9258	19750804 <--
NL 175789	B	19840801		
NL 175789	C	19850102		
DK 7503564	A	19760207	DK 1975-3564	19750805 <--
DK 155088	B	19890206		
DK 155088	C	19890626		
SE 7508829	A	19760209	SE 1975-8829	19750805 <--
SE 427030	B	19830228		
SE 427030	C	19830609		
ES 440032	A1	19770601	ES 1975-440032	19750805 <--
CH 617668	A	19800613	CH 1975-10202	19750805 <--
HU 176016	P	19801128	HU 1975-SI1485	19750805 <--
BE 832190	A1	19751201	BE 1975-158997	19750806 <--
FR 2281131	A1	19760305	FR 1975-24559	19750806 <--
FR 2281131	B1	19800418		
DD 119213	C	19760412	DD 1975-187724	19750806 <--
AU 7583734	A1	19770210	AU 1975-83734	19750806 <--
GB 1511669	A	19780524	GB 1975-32916	19750806 <--
US 4076702	A	19780228	US 1976-716265	19760820 <--
US 4076703	A	19780228	US 1976-716266	19760820 <--
US 4076704	A	19780228	US 1976-716267	19760820 <--
US 4076705	A	19780228	US 1976-716268	19760820 <--
ES 455504	A1	19780116	ES 1977-455504	19770131 <--
ES 455505	A1	19780116	ES 1977-455505	19770131 <--
ES 455506	A1	19780116	ES 1977-455506	19770131 <--
ES 455507	A1	19780116	ES 1977-455507	19770131 <--
US 4240957	A	19801223	US 1977-775646	19770307 <--
US 4154727	A	19790515	US 1978-867605	19780106 <--
CH 627438	A	19820115	CH 1979-4617	19790517 <--
CH 627439	A	19820115	CH 1979-4618	19790517 <--
CH 627440	A	19820115	CH 1979-8270	19790912 <--
PRIORITY APPLN. INFO.:			JP 1974-90565 A	19740806
			JP 1974-90566 A	19740806
			US 1975-601134 A3	19750801
			CH 1975-10202 A	19750805

GI



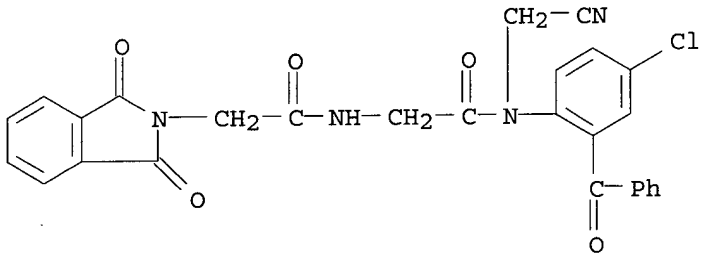
I

AB The title compds. I [e.g., R1 = H, phthalyl, PhCH2O2C, Me, Ph3C, ClCH2CO, PhCH2CH2; R2 = H, Me; R3,R4 = H, Cl, F, 2-ClC6H4CO, Bz, 2-FC6H4CO] and phenylalanylglycine anilide analog (.apprx.50 compds.), useful as sedatives and muscle relaxants with LD50 of >1000 mg/kg orally in mice, were prepared by 5 different methods. Thus, e.g., treatment of Ph3C-Gly-Gly with SOCl2 followed by addition of 2,5-(H2N)ClC6H4COPh and detritylation gave I (R1 = R2 = H, R3 = Bz, R4 = Cl).

IT **59180-22-2P 59180-23-3P 59180-25-5P 59180-27-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

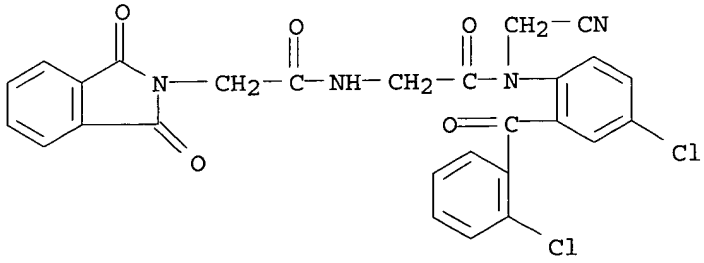
RN 59180-22-2 HCAPLUS

CN 2H-Isoindole-2-acetamide, N-[2-[(2-benzoyl-4-chlorophenyl)(cyanomethyl)amino]-2-oxoethyl]-1,3-dihydro-1,3-dioxo- (9CI) (CA INDEX NAME)



RN 59180-23-3 HCAPLUS

CN 2H-Isoindole-2-acetamide, N-[2-[[4-chloro-2-(2-chlorobenzoyl)phenyl](cyanomethyl)amino]-2-oxoethyl]-1,3-dihydro-1,3-dioxo- (9CI) (CA INDEX NAME)

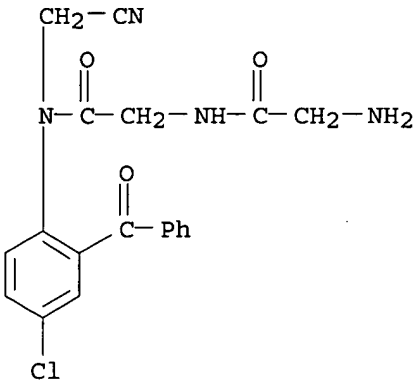


RN 59180-25-5 HCAPLUS

CN Glycinamide, glycyl-N-(2-benzoyl-4-chlorophenyl)-N-(cyanomethyl)-, 2-hydroxy-1,2,3-propanetricarboxylate (2:1) (9CI) (CA INDEX NAME)

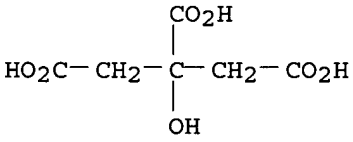
CM 1

CRN 59180-24-4
CMF C19 H17 Cl N4 O3



CM 2

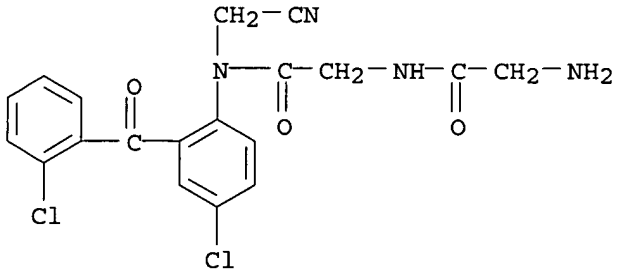
CRN 77-92-9
CMF C6 H8 O7



RN 59180-27-7 HCAPLUS
CN Glycinamide, glycyl-N-[4-chloro-2-(2-chlorobenzoyl)phenyl]-N-(cyanomethyl)-, 2-hydroxy-1,2,3-propanetricarboxylate (2:1) (9CI) (CA INDEX NAME)

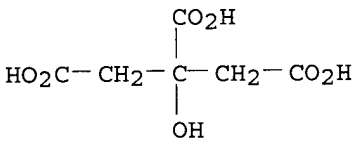
CM 1

CRN 59180-26-6
CMF C19 H16 Cl2 N4 O3



CM 2

CRN 77-92-9
CMF C6 H8 O7



L12 ANSWER 36 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1972:434570 HCAPLUS
DOCUMENT NUMBER: 77:34570
TITLE: Pyrazinamide derivatives as diuretics and natriuretics
INVENTOR(S): Cragoe, Edward J., Jr.; Shepard, Kenneth L.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: Fr. Demande, 54 pp.
CODEN: FRXXBL
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

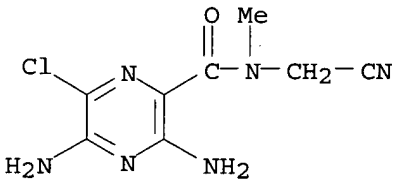
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2034542		19710108		<--
PRIORITY APPLN. INFO.:			US 1969-798809	19690212

GI For diagram(s), see printed CA Issue.

AB Refluxing a mixture of I (R1 = Me, R2 = R3 = H, R4 = Cl), 5% aqueous NaOH, and iso-PrOH for 1 hr gave the carboxylic acid I (R1 = R2 = R3 = H, R4 = Cl) (II). A mixture of CH.tplbond.CCH2NH2, Me 3-amino-5,6-dichloropyrazinoate, and Me2SO when stirred for 1 hr gave I (R1 = Me, R2 = H, R3 = CH.tplbond.CCH2, R4 = Cl) which on hydrolysis gave the corresponding carboxylic acid, R1 = H. Using similar methods, 21 I were prepared in which R1 = H, R2 = H, Me, allyl, cyclopentyl, Me2NCH2CH2, 2-furylmethyl, MeO, NH2, etc., R3 = H or Me, R4 = Cl, Br, or iodo. To a solution of II, Et3N, and Me2NCHO was added N-tert-butyl-5-methylisoxazolium perchlorate (III) and the mixture stirred 2 hr to give IV (R2 = R3 = H, R4 = Cl, R5 = Me, R6 = Me3C) (V). Nineteen IV were similarly prepared in which R2 = H, allyl, propargyl, cyclopentyl, hydroxyalkyl, benzyl, furylmethyl, phenyl, substituted phenyl, MeO, NH2, Me, or Et; R3 = H or Me; R4 = Cl, Br, or iodo; R5 = Me or Ph; R6 = Et, CMe3, or Me. Re-fluxing a mixture of 1-aminopyrrolidine and V for 2 hr gave VI (R2 = R3 = H, R4 = Cl, R1 = pyrrolidino) as a high m.p. solid. Twenty-two VI were similarly prepared in which R2, R3, and R4 were as in V and R1 was a group such as MePrN(CH2)2, MeOCH2CH2, benzyl, Me2NCH2CH2, pyrrolidinoethyl, and 1-methyl-4-piperazinoethyl. VI (R2 = R3 = H, R4 = Cl, R1 = 2-pyridylamino) was prepared by refluxing a mixture of 2-hydrazinopyridine (VII) and MeCN. Reacting III, 3,5-diamino-6-chloropyrazinoic acid (VIII) with Et3N in Me2NCHO, then addition of 2-hydrazinopyrimidine in DMF and further heating gave VI (R2 = R3 = H, R4 = Cl, R1 = 2-pyrimidinylamino). In THF, under similar conditions were prepared a further 14 amides and hydrazines VI including VI (R2 = R3 = H, R4 = Cl, R1 = 4H-1,2,4-triazolyl). Stirring a mixture of benzamidine and VII in H2O for 2 hr gave IX. Five analogs were prepared using other amidines. In a similar manner using guanidine in place of benzamidine was prepared X (R = H) (XI) giving a crystalline hydrochloride.

XI could also be prepared directly from VIII without isolation of intermediates. By similar methods were prepared X (R = OH, CH2Ph) and 39 analogs of X in which the NH2 adjacent to the Cl could also be substituted. With aminoguanidine and 2-hydrazino-2-imidazoline were prepared X (R = NH2 and 2-aminoimidazoline). A mixture of CNNH2 and Na in iso-PrOH was refluxed for 0.5 hr and then heated with N-tert-butyl-3-(3,5-diamino-6-chloropyrazinylcarbonyloxy)crotonamide to give N-cyano-3,5-diamino-6-chloropyrazinecar-boxamide. Refluxing N-tert-butyl-3-methyl-3-(3,5-diamino-6-chloropyrazinylcarbonyloxy)acrylamide (XII) and benzyloxydiguanide in THF gave XIII (R = H, R1 = CH2Ph). Twelve XI in which R was H and R1 1-6C alkyl, or R was a substituent such as cyclopentyl, PhCH2, and furylmethyl, and R1 was substituted benzyl were prepared Refluxing a mixture of 2-amino-2-thiazoline, XII, and THF gave N-(2-thiazolin-2-yl)-3,5-diamino-6-chloropyrazinecarboxamide (XIV, R = R1 = R2 = R3 = H). Three analogs were prepared in which R was cyclopentyl, benzyl and HO(CH2)2, the other substituents being H, Me, or C6H13. XIV where RNH was pyrrolidino was also prepared The 4- and 2-pyridyl groups and 2-pyrimidinyl could be substituted for the thiazoline. Reaction of V with sulfamide and Et3N in MeCN at room-temperature gave XV (R = R1 = R2 = H, X = Cl). Eighteen XV were similarly prepared Properties are also given for a further 19 amides XVI. containing a wide variety of substituents. The products are useful in treatment of hypertension and related conditions by causing diuresis without elimination of potassium. Daily doses are 5 mg-1 g.

IT **33214-77-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 33214-77-6 HCAPLUS
CN Pyrazinecarboxamide, 3,5-diamino-6-chloro-N-(cyanomethyl)-N-methyl- (8CI) (CA INDEX NAME)



L12 ANSWER 37 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1971:420438 HCAPLUS
DOCUMENT NUMBER: 75:20438
TITLE: N-substituted 3,5-diamino-6-halopyrazinamides
INVENTOR(S): Shepard, Kenneth L.; Cragoe, Edward J., Jr.
PATENT ASSIGNEE(S): Merck and Co., Inc.
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3573306	A	19710330	US 1969-804663	19690305 <--
NL 7001141	A	19700908	NL 1970-1141	19700127 <--
BE 746816	A	19700904	BE 1970-746816	19700304 <--

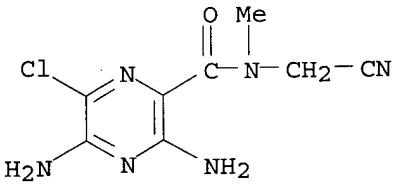
PRIORITY APPLN. INFO.: US 1969-804663 A 19690305

AB Addition of diphenylcarbamoyl chloride to 3,5-diamino-6-chloropyrazinoic acid and Et3N in HCONMe2 gave 3,5-diamino-6-chloropyrazinecarboxylic diphenylcarbamic anhydride (I). Refluxing Na in iso-PrOH with guanidine-HCl and addition of I gave 1-(3,5-diamino-6-chloropyrazinoyl)guanidine. Similarly prepared were 1,1,3,3-tetramethyl-2-(3,5-diamino-6-chloropyrazinoyl)guanidine, 1-(3,5-diamino-6-chloropyrazinoyl)-3-cyanoguanidine, N-methyl-N-(cyanomethyl)-3,5-diamino-6-chloropyrazinecarboxamide, N-(2,2-diethoxyethyl)-3,5-diamino-6-chloropyrazinecarboxamide, N-(2-morpholinoethyl)-3,5-diamino-6-chloropyrazinecarboxamide, N-(4-pyridylmethyl)-3,5-diamino-6-chloropyrazinecarboxamide, N-(2-pyridyl)-3,5-diamino-6-chloropyrazinecarboxamide, 3,5-diamino-6-chloropyrazinecarboxylic acid 1,2-dimethylhydrazide, 3,5-diamino-6-chloropyrazinecarboxylic acid 1-methyl-2-benzylidenehydrazide, and N-(3,5-diamino-6-chloropyrazinoyl)morpholine. These compds. had diuretic activity at 10-100 mg.

IT **33214-77-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 33214-77-6 HCAPLUS

CN Pyrazinecarboxamide, 3,5-diamino-6-chloro-N-(cyanomethyl)-N-methyl- (8CI) (CA INDEX NAME)



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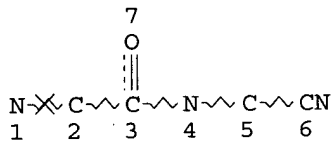
L1 STR



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NSPEC IS RC AT 2
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 7

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STEREO ATTRIBUTES: NONE
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L6               STR
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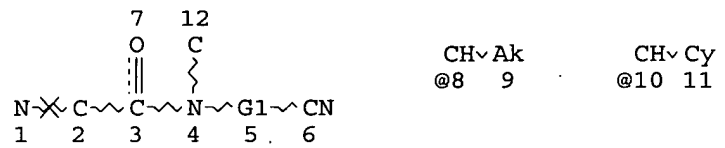


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NSPEC   IS RC     AT   2
NSPEC   IS RC     AT  12
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  12

STEREO ATTRIBUTES: NONE
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L9        359971 SEA FILE=HCAPLUS ABB=ON  PLU=ON  DIABETE?/CV OR (HYPERGLYCEMIA/
                 CV OR GLUCEMIA/CV OR "GLYCEMIA OR GLUCEMIA"/CV OR "HIGH BLOOD
                 GLUCOSE"/CV OR "HIGH BLOOD SUGAR"/CV OR "ANTIDIABETIC AGENTS"/C
                 V OR "DIABETES MELLITUS"/CV OR GLUCOSE/CV OR INSULIN/CV) OR
                 ?DIABET? OR (BLOOD OR BLD)(W)(GLUCOSE OR SUGAR) OR ?GLUCEM? OR
                 ?GLYCEM?
L10            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 AND L9
L11           49 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L8 NOT L10
L12           37 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11 AND PD=<OCTOBER 23, 2002
L13         3801 SEA FILE=REGISTRY ABB=ON  PLU=ON  L5 NOT L7
L14          338 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L13
L15          322 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L14 NOT (L10 OR L12)
L16           18 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L15 AND L9
L17            5 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L16 AND PD=<OCTOBER 23, 2002


=>
=>

=> d ibib abs hitstr l17 1-5

L17  ANSWER 1 OF 5  HCAPLUS  COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER:         2001:176761  HCAPLUS
DOCUMENT NUMBER:          134:217203
TITLE:                    Amide compounds as inhibitors for fat accumulation
INVENTOR(S):              Tachikawa, Nobuko; Otsubo, Tsuguaki; Murakami, Hiroko
PATENT ASSIGNEE(S):       Sumitomo Pharmaceuticals Co., Ltd., Japan; Sumitomo
                          Chemical Co., Ltd.
SOURCE:                   Jpn. Kokai Tokkyo Koho, 36 pp.
                          CODEN: JKXXAF
DOCUMENT TYPE:            Patent
LANGUAGE:                 Japanese
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:
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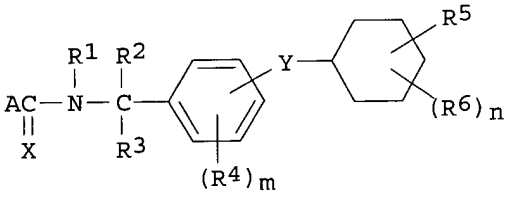
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001064176	A2	20010313	JP 1999-237907	19990825 <--
PRIORITY APPLN. INFO.:			JP 1999-237907	19990825
OTHER SOURCE(S):	MARPAT 134:217203			

GI



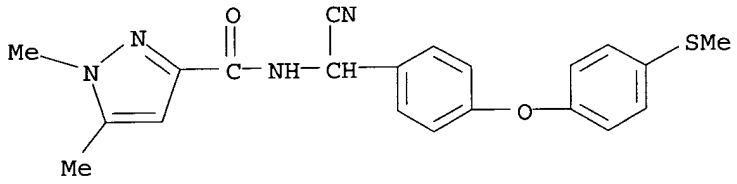
I

AB Amide compds. (I; R1,R2,R4,R4 = H, C1-4 alkyl, etc.; R5 = H, OH, etc.; R6 = H, C3-6 cycloalkyl, etc.; m = 1,2; n = 1-4; A = pyrazol-5-yl, etc.; X,Z = O, S; Y = O, S, etc.; B = benzene, pyridine ring) and their pharmaceutically acceptable salts are claimed as inhibitors for fat accumulation and are useful as antiobesity, **antidiabetic**, and hypolipidemic drugs.

IT **132528-39-3 132528-40-6 132528-41-7 132548-61-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(amide compds. as inhibitors for fat accumulation)

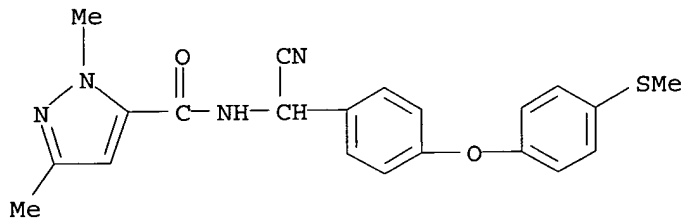
RN 132528-39-3 HCAPLUS

CN 1H-Pyrazole-3-carboxamide, N-[cyano[4-[4-(methylthio)phenoxy]phenyl]methyl]-1,5-dimethyl- (9CI) (CA INDEX NAME)

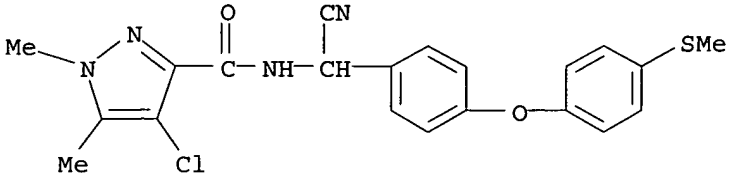


RN 132528-40-6 HCAPLUS

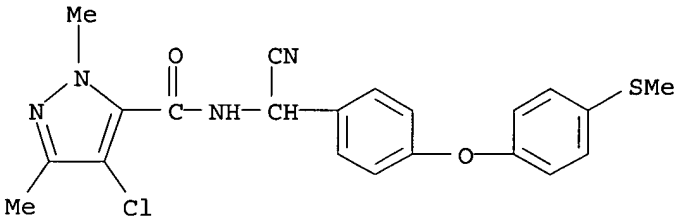
CN 1H-Pyrazole-5-carboxamide, N-[cyano[4-[4-(methylthio)phenoxy]phenyl]methyl]-1,3-dimethyl- (9CI) (CA INDEX NAME)



RN 132528-41-7 HCAPLUS
CN 1H-Pyrazole-3-carboxamide, 4-chloro-N-[cyano[4-[4-(methylthio)phenoxy]phenyl]methyl]-1,5-dimethyl- (9CI) (CA INDEX NAME)



RN 132548-61-9 HCAPLUS
CN 1H-Pyrazole-5-carboxamide, 4-chloro-N-[cyano[4-[4-(methylthio)phenoxy]phenyl]methyl]-1,3-dimethyl- (9CI) (CA INDEX NAME)



L17 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:628128 HCAPLUS
DOCUMENT NUMBER: 133:208196
TITLE: Preparation of peptides as reversible inhibitors of cathepsin S
INVENTOR(S): Cywin, Charles L.; Frye, Leah L.; Morwick, Tina; Spero, Denice M.; Thomson, David; Ward, Yancey
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 315 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000051998	A1	20000908	WO 1999-US26278	19991105 <--
W: CA, JP, MX				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2360740	AA	20000908	CA 1999-2360740	19991105 <--
EP 1159273	A1	20011205	EP 1999-973745	19991105 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6395897	B1	20020528	US 1999-434106	19991105 <--
JP 2002538151	T2	20021112	JP 2000-602225	19991105
US 6608057	B2	20030819	US 2001-82952	20011024
US 2002091259	A1	20020711	US 2002-82952	20020224 <--
US 2003158406	A1	20030821	US 2003-366282	20030213
US 6730671	B2	20040504		

PRIORITY APPLN. INFO.:

US 1999-122570P	P	19990302
US 1999-434106	A1	19991105
WO 1999-US26278	W	19991105
US 2001-82952	A3	20011024

OTHER SOURCE(S): MARPAT 133:208196

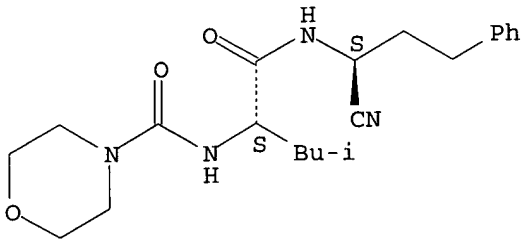
AB Compds. R1-A-NHCR2R3C(:X)NR4CR5R6R7 [A = C:O, C:S, C:NH or substituted imino group; R1 = (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl, amino; R2, R4 = H, alkyl; R3, R6 = H or (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl, heteroaryl; R5 = H, alkyl, cycloalkyl; R7 = R8C(Z), where Z = O, S, NH or substituted derivative and R8 is (un)substituted 5-8 membered monocyclic or 8-11 membered bicyclic heteroaryl having 1-4 heteroatoms selected from N, O and S; X = O, S, NOH] were prepared as cathepsin S inhibitors. Thus, morpholine-4-carboxylic acid [1-(S)-[1-(S)-cyano-3-phenylpropylcarbamoyl]-3-methylbutyl]amide was prepared by coupling L-homophenylalaninamide with N-(4-morpholinecarbonyl)-L-leucine and reaction with cyanuric chloride. Compds. of the invention were evaluated for inhibition of cathepsin S (IC50 ≤ 100 μM).

IT **290816-49-8P 290816-51-2P 290816-76-1P**
290816-77-2P 290816-78-3P 290816-79-4P
290816-81-8P 290816-82-9P 290816-83-0P
290816-84-1P 290816-85-2P 290816-86-3P
290816-87-4P 290816-88-5P 290816-89-6P
290816-90-9P 290816-91-0P 290816-92-1P
290816-93-2P 290816-94-3P 290816-95-4P
290816-96-5P 290816-97-6P 290817-01-5P
290817-02-6P 290817-03-7P 290817-07-1P
290817-08-2P 290817-09-3P 290817-10-6P
290817-11-7P 290817-12-8P 290817-14-0P
290817-15-1P 290817-17-3P 290817-18-4P
290817-19-5P 290817-20-8P 290817-21-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of peptides as reversible inhibitors of cathepsin S)

RN 290816-49-8 HCAPLUS

CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1-cyano-3-phenylpropyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

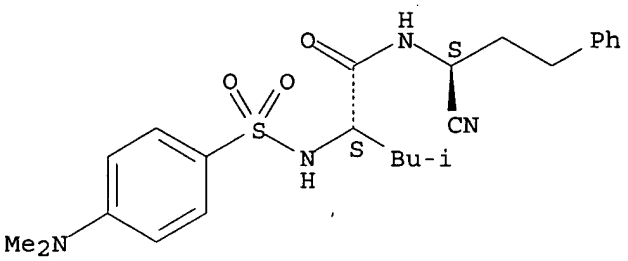
Absolute stereochemistry.



RN 290816-51-2 HCAPLUS

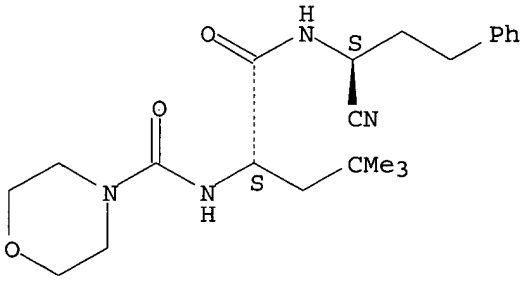
CN Pentanamide, N-[(1S)-1-cyano-3-phenylpropyl]-2-[[[4-(dimethylamino)phenyl]sulfonyl]amino]-4-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



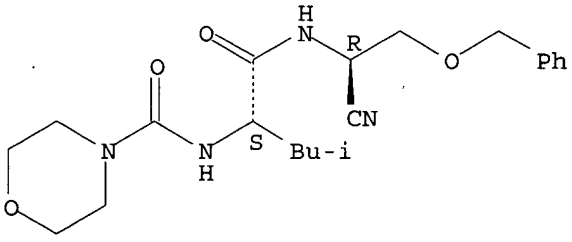
RN 290816-76-1 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1-cyano-3-phenylpropyl]amino]carbonyl]-3,3-dimethylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



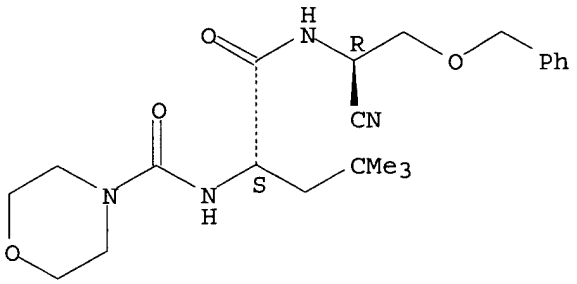
RN 290816-77-2 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



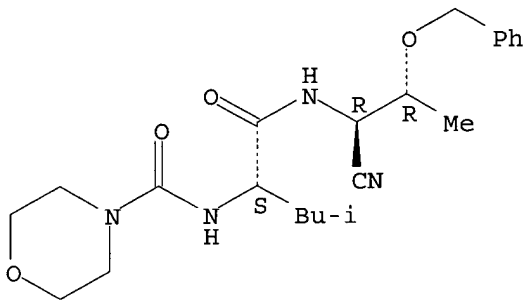
RN 290816-78-3 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3,3-dimethylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



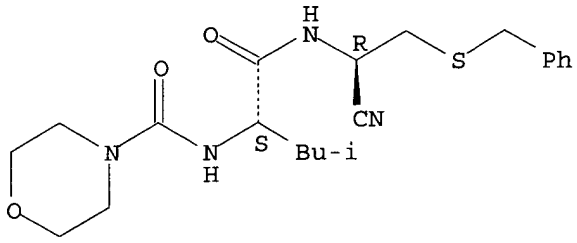
RN 290816-79-4 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R,2R)-1-cyano-2-(phenylmethoxy)propyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



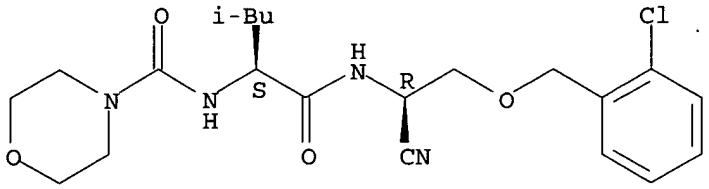
RN 290816-81-8 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(phenylmethyl)thio]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



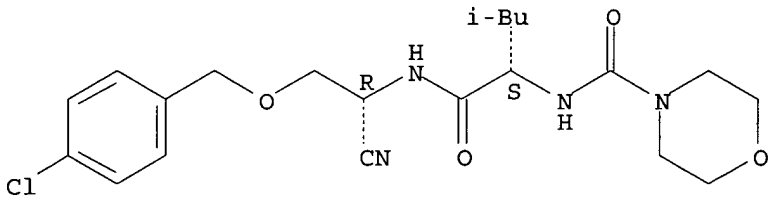
RN 290816-82-9 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-2-[(2-chlorophenyl)methoxy]-1-cyanoethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



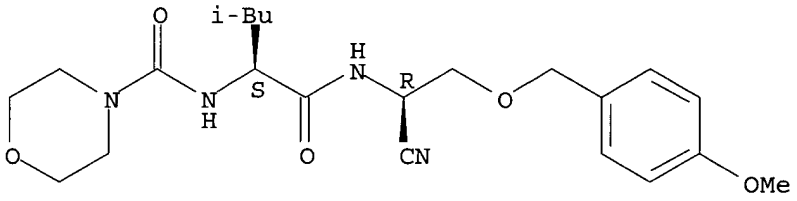
RN 290816-83-0 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-2-[(4-chlorophenyl)methoxy]-1-cyanoethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



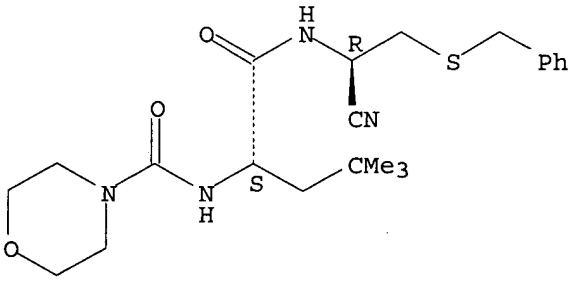
RN 290816-84-1 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(4-methoxyphenyl)methoxy]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



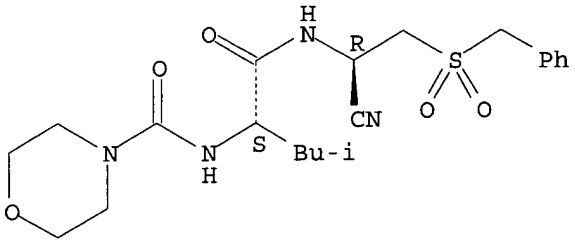
RN 290816-85-2 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(phenylmethyl)thio]ethyl]amino]carbonyl]-3,3-dimethylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



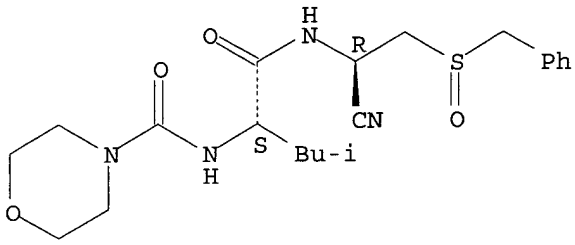
RN 290816-86-3 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(phenylmethyl)sulfonyl]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



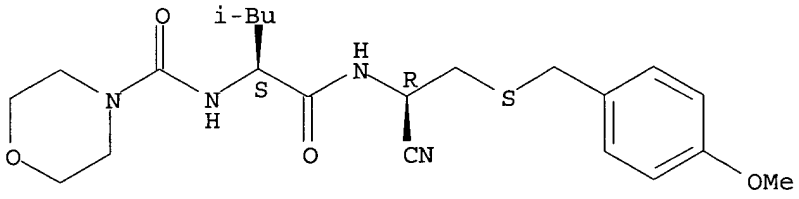
RN 290816-87-4 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(phenylmethyl)sulfinyl]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



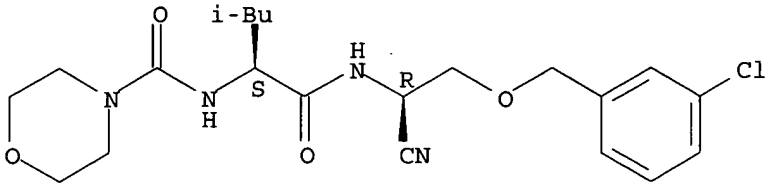
RN 290816-88-5 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[[(4-methoxyphenyl)methyl]thio]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



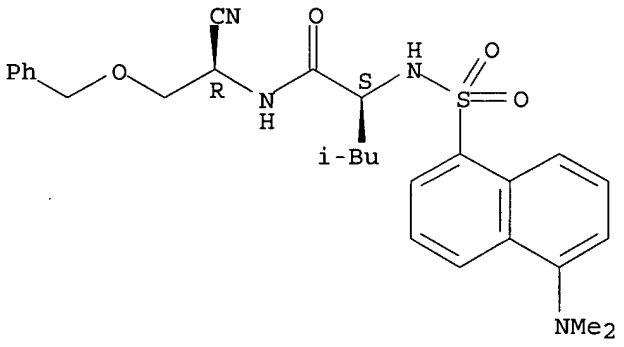
RN 290816-89-6 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-2-[(3-chlorophenyl)methoxy]-1-cyanoethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



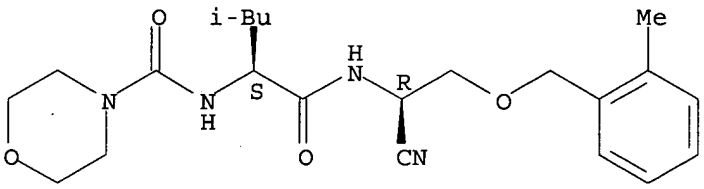
RN 290816-90-9 HCAPLUS
CN Pentanamide, N-[(1R)-1-cyano-2-(phenylmethoxy)ethyl]-2-[[[5-(dimethylamino)-1-naphthalenyl]sulfonyl]amino]-4-methyl-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



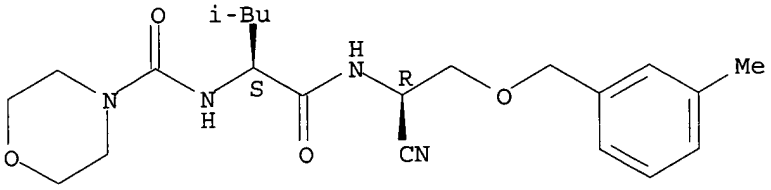
RN 290816-91-0 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(2-methylphenyl)methoxy]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



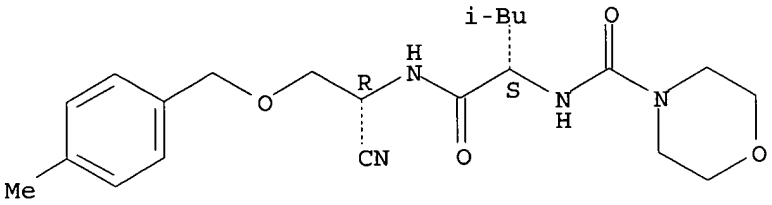
RN 290816-92-1 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(3-methylphenyl)methoxy]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



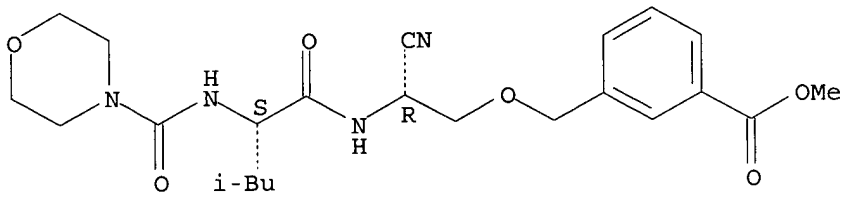
RN 290816-93-2 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1R)-1-cyano-2-[(4-methylphenyl)methoxy]ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



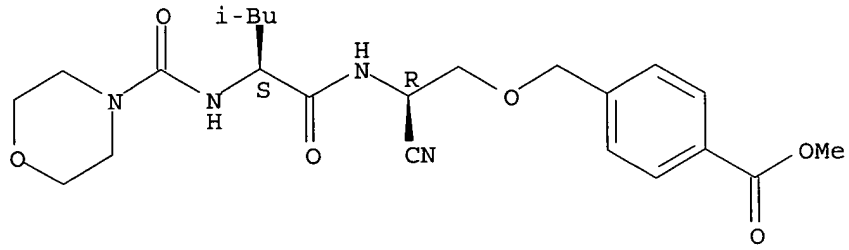
RN 290816-94-3 HCAPLUS
CN Benzoic acid, 3-[[(2R)-2-cyano-2-[[(2S)-4-methyl-2-[(4-morpholinylcarbonyl)amino]-1-oxopentyl]amino]ethoxy]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



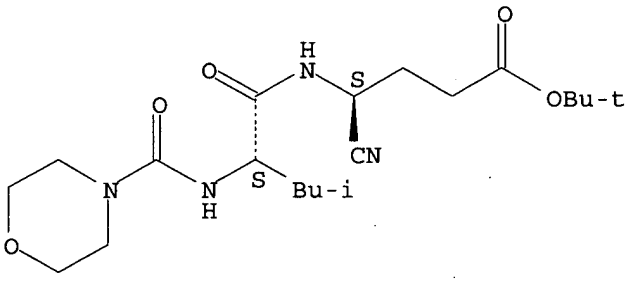
RN 290816-95-4 HCAPLUS
CN Benzoic acid, 4-[[(2R)-2-cyano-2-[[(2S)-4-methyl-2-[(4-morpholinylcarbonyl)amino]-1-oxopentyl]amino]ethoxy]methyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



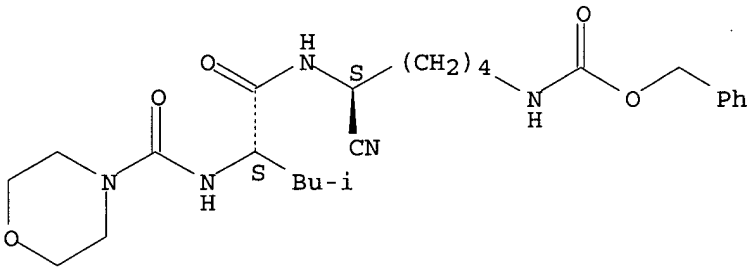
RN 290816-96-5 HCAPLUS
CN Butanoic acid, 4-cyano-4-[[(2S)-4-methyl-2-[(4-morpholinylcarbonyl)amino]-1-oxopentyl]amino]-, 1,1-dimethylethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



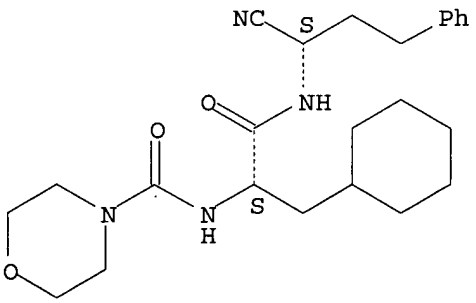
RN 290816-97-6 HCAPLUS
CN Carbamic acid, [(5S)-5-cyano-5-[[(2S)-4-methyl-2-[(4-morpholinylcarbonyl)amino]-1-oxopentyl]amino]pentyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



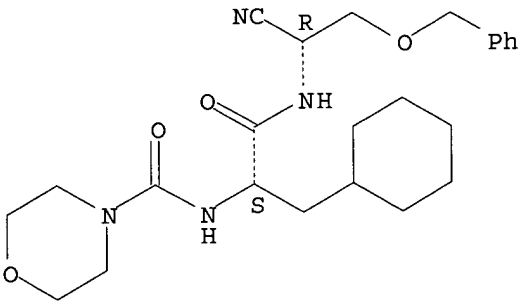
RN 290817-01-5 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-2-[[(1S)-1-cyano-3-phenylpropyl]amino]-1-(cyclohexylmethyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



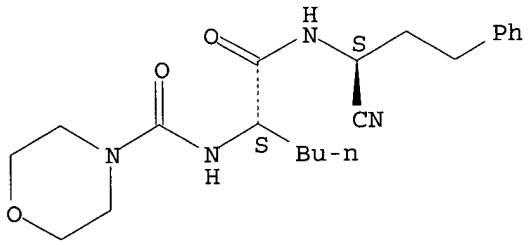
RN 290817-02-6 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-2-[[(1R)-1-cyano-2-(phenylmethoxy)ethyl]amino]-1-(cyclohexylmethyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



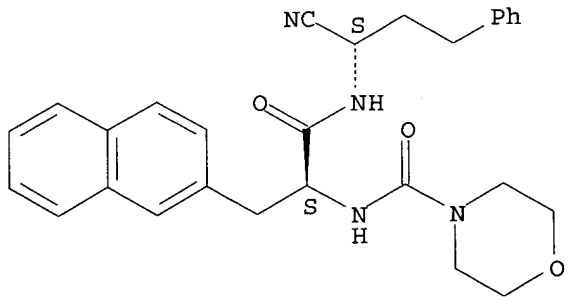
RN 290817-03-7 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1-cyano-3-phenylpropyl]amino]carbonyl]pentyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



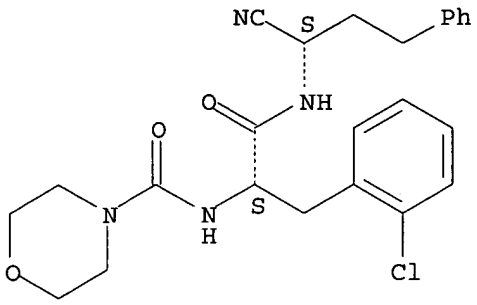
RN 290817-07-1 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-2-[[(1S)-1-cyano-3-phenylpropyl]amino]-1-(2-naphthalenylmethyl)-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



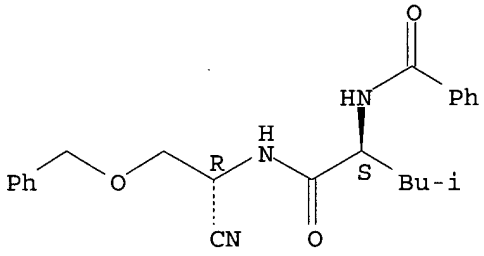
RN 290817-08-2 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[(2-chlorophenyl)methyl]-2-[[(1S)-1-cyano-3-phenylpropyl]amino]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



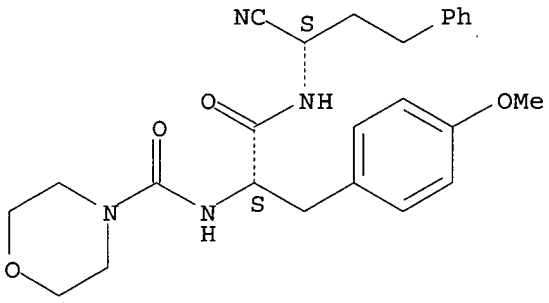
RN 290817-09-3 HCAPLUS
CN Benzamide, N-[(1S)-1-[[[(1R)-1-cyano-2-(phenylmethoxy)ethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



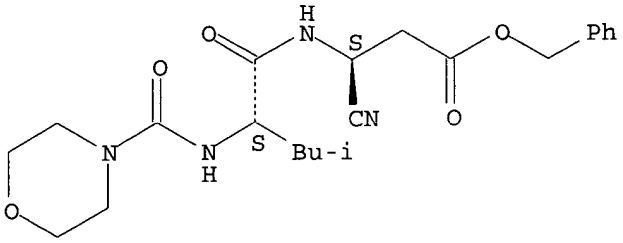
RN 290817-10-6 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-2-[[(1S)-1-cyano-3-phenylpropyl]amino]-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



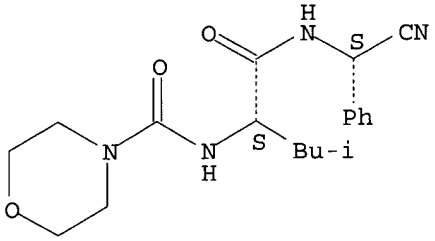
RN 290817-11-7 HCAPLUS
CN Propanoic acid, 3-cyano-3-[[(2S)-4-methyl-2-[(4-morpholinylcarbonyl)amino]-1-oxopentyl]amino]-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



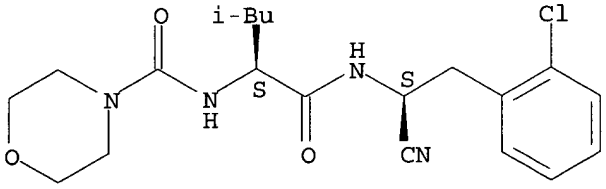
RN 290817-12-8 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(S)-cyanophenylmethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



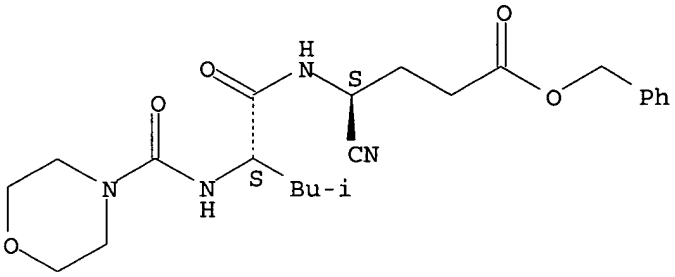
RN 290817-14-0 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-2-(2-chlorophenyl)-1-cyanoethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



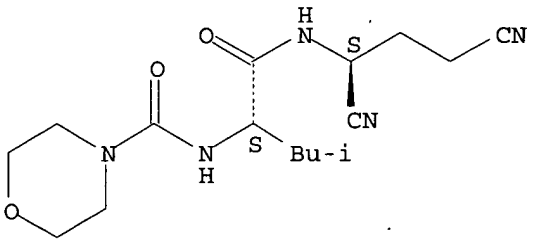
RN 290817-15-1 HCAPLUS
CN Butanoic acid, 4-cyano-4-[[(2S)-4-methyl-2-[(4-morpholinylcarbonyl)amino]-1-oxopentyl]amino]-, phenylmethyl ester, (4S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



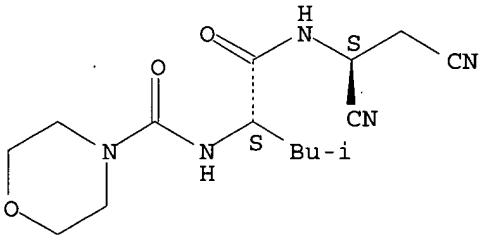
RN 290817-17-3 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1,3-dicyanopropyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



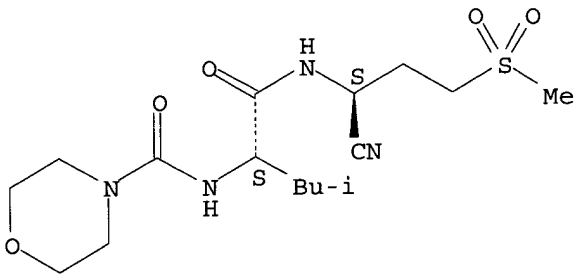
RN 290817-18-4 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1,2-dicyanoethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



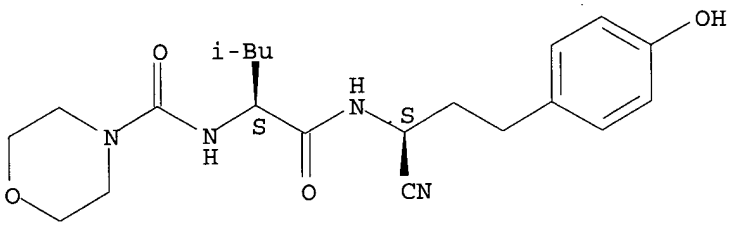
RN 290817-19-5 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1-cyano-3-(methylsulfonyl)propyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



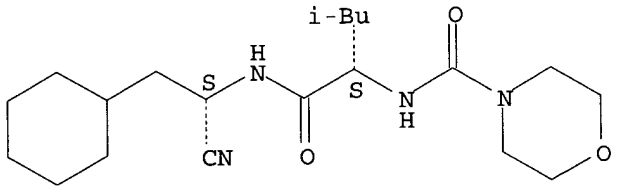
RN 290817-20-8 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1-cyano-3-(4-hydroxyphenyl)propyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 290817-21-9 HCAPLUS
CN 4-Morpholinecarboxamide, N-[(1S)-1-[[[(1S)-1-cyano-2-cyclohexylethyl]amino]carbonyl]-3-methylbutyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



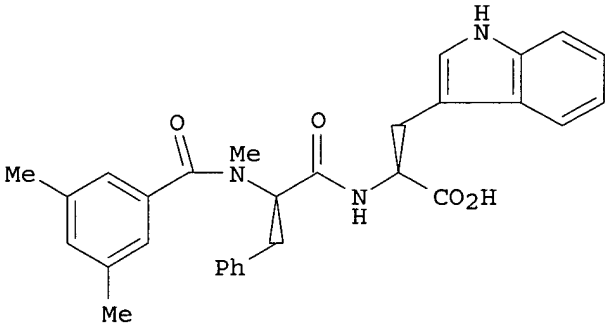
REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:887871 HCAPLUS
DOCUMENT NUMBER: 123:340965
TITLE: Preparation of dipeptide analogs as endothelin receptor antagonists.
INVENTOR(S): Saika, Hideyuki; Murata, Toshiki; Pitterna, Thomas; Frueh, Thomas; Svensson, Lene D.; Urade, Yoshihiro; Yamamura, Takaki; Okada, Toshikazu
PATENT ASSIGNEE(S): Japat Ltd., Switz.; Ciba-Geigy Japan Ltd.
SOURCE: PCT Int. Appl., 115 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent

LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9512611	A1	19950511	WO 1994-EP3418	19941017 <--
W: AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, JP, KG, KP, KR, KZ, LK, LR, LT, LV, MD, MG, MN, NO, NZ, PL, RO, RU, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
CA 2173875	AA	19950511	CA 1994-2173875	19941017 <--
AU 9478565	A1	19950523	AU 1994-78565	19941017 <--
AU 691201	B2	19980514		
EP 728145	A1	19960828	EP 1994-929557	19941017 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
BR 9407933	A	19961126	BR 1994-7933	19941017 <--
JP 09504302	T2	19970428	JP 1994-512982	19941017 <--
RU 2126418	C1	19990220	RU 1996-112148	19941017 <--
ZA 9408541	A	19950502	ZA 1994-8541	19941031 <--
FI 9601804	A	19960430	FI 1996-1804	19960426 <--
NO 9601725	A	19960429	NO 1996-1725	19960429 <--
US 5780498	A	19980714	US 1996-637720	19960430 <--
PRIORITY APPLN. INFO.:			EP 1993-810760 A	19931101
			WO 1994-EP3418 W	19941017

OTHER SOURCE(S): MARPAT 123:340965
GI



I

AB R1CONR2CH(CR3R31R311)C(X)YCHR4R5 [R1 = alkyl, cycloalkylalkyl, aralkyl, cycloalkyl, aryl, arylcycloalkyl, alkoxy, aryloxy, heteroaryl; R2 = H, alkyl, cycloalkyl, cycloalkylalkyl; R3, R31 = H, alkyl, cycloalkyl, aralkyl, aryl, heteroaryl; R3R31 = atoms to form a ring; R311 = H, alkyl, aryl; R2R311 = (CH2)n, (CH2)pAr; n = 1, 2, 3; p = 0, 1, 2; Ar = (hetero)arylene; X = O, S, NH, NHOH, CH2, etc.; Y = bond, O, CH2, imino; or X = (H, OH) and Y = bond, CH2; R4 = (CH2)sAr1; s = 0, 1, 2, 3; Ar1 = (hetero)aryl; R5 = H, carboxy, (substituted) carboxamido, PO(OH)2, tetrazolyl, CH2OH, CN], were prepared Thus, title compound (I), prepared by solution phase means, inhibited endothelin-3 induced contraction of guinea pig trachea with pA2 = 6.3. Drug formulations containing I are given.

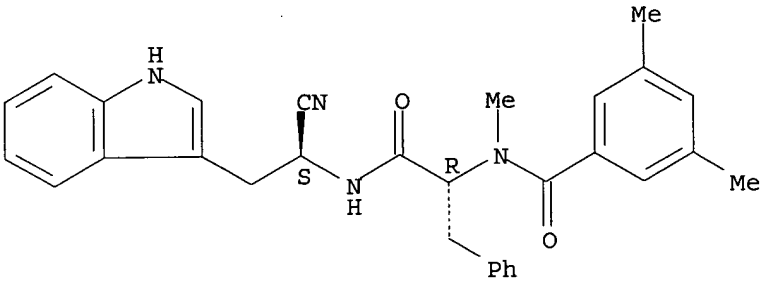
IT **169544-80-3P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dipeptide analogs as endothelin receptor antagonists)

RN 169544-80-3 HCAPLUS

CN Benzenepropanamide, N-[1-cyano-2-(1H-indol-3-yl)ethyl]-α-[(3,5-dimethylbenzoyl)methylamino]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



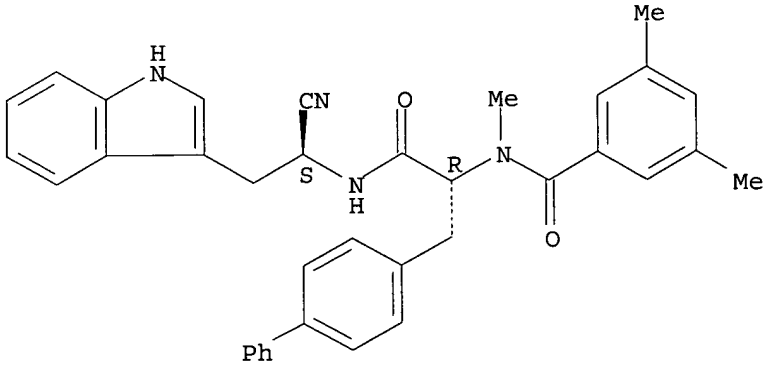
IT **169547-55-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dipeptide analogs as endothelin receptor antagonists)

RN 169547-55-1 HCAPLUS

CN [1,1'-Biphenyl]-4-propanamide, N-[1-cyano-2-(1H-indol-3-yl)ethyl]-α-[(3,5-dimethylbenzoyl)methylamino]-, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 4 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1984:628001 HCAPLUS

DOCUMENT NUMBER: 101:228001

TITLE: Amine metabolism and monoamine oxidase in liver diseases

AUTHOR(S): Kai, Yuichi

CORPORATE SOURCE: Fac. Med., Kagoshima Univ., Kagoshima, 890, Japan

SOURCE: Kagoshima Daigaku Igaku Zasshi (**1984**), 36(1), 27-67
CODEN: KDIZAA; ISSN: 0368-5063

DOCUMENT TYPE: Journal

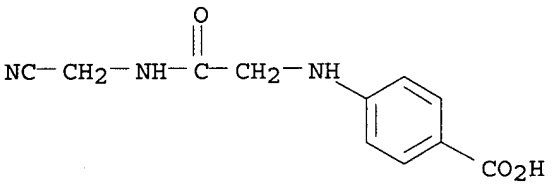
LANGUAGE: Japanese

AB Abnormal amine metabolism and changes in monoamine oxidase (MAO) activities in pathol. conditions were examined clin. and exptl. Increases in blood amine levels were seen in liver diseases and **diabetes** mellitus but not in hyperthyroidism or systemic lupus erythematosus. Serum MAO activity increased significantly in the active stage of chronic hepatitis, hepatic cirrhosis and fulminant hepatitis and in some hepatoma cases. Ammonium chloride loading in chronic hepatitis caused significant increases in total blood amines, but such increases were suppressed when polyene phosphatidylcholine was given simultaneously. L-DOPA administration did not alter total blood amines and serum MAO in chronic liver diseases. MAO activity was separated into 3 bands on starch gel electrophoresis at pH 8.4. Fraction I migrated with albumin, fraction II migrated with α2- and β-globulin, and fraction III migrated with γ-globulin. MAO in normal subjects and patients with fulminant hepatitis was found in II, and MAO in patients with chronic hepatitis or liver cirrhosis was found in I. When N-(N-p-carboxyphenylglycyl)aminoacetonitrile, a lathyrogen, was administered for 4 wk to patients with chronic hepatitis or liver cirrhosis having high MAO in serum, MAO in I decreased. When a steroid hormone was administered to rats in the convalescent stage of chronic damage induced by CCl4, total amines in blood, in urine, and in the liver decreased. Acute EtOH poisoning in rats caused increase in total amines in blood and MAO in serum and liver. In vitro expts. showed that EtOH at high concns. inhibited serum and liver MAO.

IT **19065-92-0**
RL: BIOL (Biological study)
(monoamine oxidase of blood serum response to, in liver diseases)

RN 19065-92-0 HCAPLUS

CN Benzoic acid, 4-[[2-[(cyanomethyl)amino]-2-oxoethyl]amino]- (9CI) (CA INDEX NAME)



L17 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1932:49151 HCAPLUS
DOCUMENT NUMBER: 26:49151
ORIGINAL REFERENCE NO.: 26:5071f-i,5072a-c
TITLE: Syntheses of derivatives of amino acids
AUTHOR(S): Fredenberg, Karl; Eichel, Helmut; Leutert, Fritz
SOURCE: Ber. (**1932**), 65B, 1183-91
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 26:49151

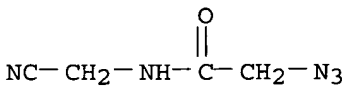
AB In connection with their work on insulin the authors have synthesized a number of amino acid derivs. by the action of α-azidoacyl chlorides on phenols and amino acids and reduction of the azido group to NH2. For the preparation of glycine Ph ester and a simple dipeptide, the reduction was effected with nascent H, but for the amino acid esters of HO acids recourse had to be had to catalytic hydrogenation. The present report is made now because Bertho and Maier likewise describe the catalytic conversion of azido compds. into the corresponding NH2 derivs. (C. A. 26, 3778). The new process is being used for various synthetic purposes, such

as the preparation of polypeptides and for the study of the imido esters and amidines of amino acids. Imidoglycine Et ester, b13 42-3°, was obtained from its HCl salt (prepared according to Curtius from ClH.H2NCH2CN with alc. 31HCl) with Na or Tl alcoholate in absolute alc., but it changes even in the cold into partly amorphous, partly crystalline polymerization products, none of which had a **hypoglycemic** action. Et benzoylaminoimidoacetate-HCl (90% yield from BzNHCH2CN in CHCl3-C6H6-EtOH with Hcl gas), decomps. around 134°; the free imido ester is a yellowish oil. With NH3 in absolute alc. 8 g. of the HCl salt gives 6 g. benzoylaminoacetamidine-Hcl, m. 184°. Et imidothiophenate-HCl, obtained in 3-g. yield from 2.2 g. α-C4H3SCN in alc. with dry Hcl, decomps. 126°, solidifies (amide) and m. 176°. Thiophenamidine-HCl m. 176°. Thiophenoylaminoacetomitrile, from C4H3SCOCl and NCCH2NH2.H2SO4 with dilute NaOH in benzene, m. 129-30°. Et thiophenoylaminoimidoacetate-Hcl, decomps.117-20°. Thiophenoylaminoacetamidine-HCl, decomps. about 275°. (Chloroacetylamino) acetonitrile, m. 90-1°; Et imidoacetate-Hcl, decomps. 122°. (Azidoacetamino)-acetonitrile, from the ClCH2CONHCH2CN with NaN3 refluxed 15 min. in 50% alc. (yield, 65%), b0.3 148-53°. Azidoacetonitrile, similarly obtained from ClCH2CN, b12 53°, deflagrates when dropped on a hot plate. (p-Toluenesulfonylamino)acetonitrile, m. 136°; acetamidine-HCl, decomps. around 185°. (α-Azidopropionyl)glycine, yellowish oil, gives with NH4OH and amalgamated Al in water dl-alanylglycine, m. 224°, whose αnaphthalenesulfonyl derivative m. 141-2°. Ph α-azidopropionate, from MeCH-(N3)COCl in CHCl3, and PhOH in pyridine (70% yield), b0.3 76°, gives alanine Ph ester-Hcl, m. 131°, in moist ether with amalgamated Al. Et (azidoacetyl)lactate (75% yield), b0.2 79°, gives with p-HOC6H4CO2H in CHCl3 suspension 65% of p-(azidoaceloxy)-benzoic acid, m. 160°. (Azidoacetyl)salicylic acid (80% yield), m. 104°; reduction with Al gave only reddish sirups; hydrogenation with Pt or Pd in alc. and water yielded large amts. of low-melting products which it was very difficult to sep.; with Pt sponge in MeOAc was obtained a product, m. 164-6°, with 7.42-8.67% N but which was not the expected glycylsalicylic acid; its equivalent weight (titration in alc. with 0.01 N NaOH) was 111.5-3.4. (Azidoacetyl)lactic acid (35% yield), m. 52°, gives with Pt sponge in water 90% of glycyllactic acid, m. 161°, which, on addition of a little alc. to its concentrated aqueous solution, seps. as a trihydrate, m. 148°; it is not attacked by pepsin. Azidoacelic anhydride, from the Ag salt and the chloride in absolute ether, b0.2 110°. Pure glycylglycine is obtained in 10-g. yield from 10 g. glycine anhydride heated with 120 cc. 10% NH4OH in a pressure flask on the water bath until no crystals sep. on cooling, then evaporating to a sirup and precipitating with MeOH.

IT **857817-74-4**, Glycinonitrile, N-α-triazoacetyl-
(preparation of)

RN 857817-74-4 HCAPLUS

CN Glycinonitrile, N-α-triazoacetyl- (3CI) (CA INDEX NAME)



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